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(FILE 'HOME' ENTERED AT 17:58:00 ON 12 APR 2005)

FILE 'REGISTRY' ENTERED AT 17:58:05 ON 12 APR 2005

L1 STRUCTURE UPLOADED
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L3 1 S L2
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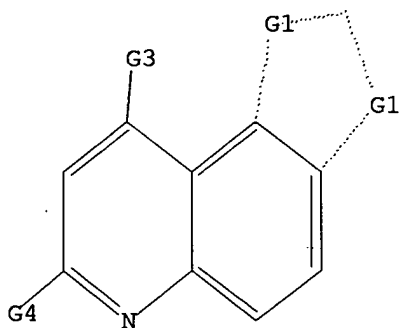
FILE 'CAPLUS' ENTERED AT 18:00:43 ON 12 APR 2005

L5 4 S L4

=> d 12

L2 HAS NO ANSWERS

L2 STR



G1 C,N

G2

G3 C,O,S,N,X,CN

G4 O,S,N,Cl,Br,F,I,CN

Structure attributes must be viewed using STN Express query preparation.

=> d 1-4 bib abs hitstr

L5 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:658121 CAPLUS

DN 137:201294

TI Preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compounds as androgen receptor modulators

IN Zhi, Lin; Van Oeveren, Cornelis Arjan; Chen, Jyun-Hung; Higuchi, Robert I.

PA Ligand Pharmaceuticals Incorporated, USA

SO PCT Int. Appl., 132 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002066475	A2	20020829	WO 2002-IB537	20020223
	WO 2002066475	A3	20030123		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
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 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 US 2002183346 A1 20021205 US 2002-80926 20020222
 CA 2434299 AA 20020829 CA 2002-2434299 20020223
 EP 1363909 A2 20031126 EP 2002-702589 20020223
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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 BR 2002007549 A 20040803 BR 2002-7549 20020223
 JP 2004524309 T2 20040812 JP 2002-565989 20020223
 PRAI US 2001-271189P P 20010223
 WO 2002-IB537 W 20020223
 OS MARPAT 137:201294
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title nonsteroidal tricyclic compds. I-VIII [wherein R1 = H, halo, NO2, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl or heteroalkyl; R2 = H, halo, Me, CF3, CHF2, CH2F, CF2Cl, CN, CF2OR12, CH2OR12, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, or alkynyl; R3-R8 = independently H, halo, OR12, NR12R13, SO0-2R12, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, (hetero)aryl, or arylalkyl; or R3R5 or R5R7 = a bond; or C2R4R6 or C2R6R8 = (un)substituted carbocyclic or heterocyclic ring; R9 and R10 = independently H, halo, CN, OR12, NR12R13, Cm(R12)2mOR13, SO0-2R12, NR12COR13, or (un)substituted (halo)alkyl, heteroalkyl, or arylalkyl; R11 = H, halo, CN, OR14, NR14R15, SO0-2R14, CH2R14, COR14, CO2R14, CONR13R14, or (un)substituted (halo)alkyl or heteroalkyl; R12 and R13 = independently H or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, or (hetero)aryl; R14 = H, COR15, CO2R15, CONR15R16, or (un)substituted (halo)alkyl, heteroalkyl, or (hetero)aryl; R15 and R16 = independently H or (un)substituted (halo)alkyl, or heteroalkyl; W = O or S; X = O, S, or NR14; Y = O, S, NR12, NOR12, or CR12R13; Z = O, S, or NR12; n = 0-2; m = 0-2; or pharmaceutically acceptable salts thereof] were prepared as modulators of androgen receptors. For example, cyclization of 6-hydrazino-4-trifluoromethylquinolin-2(1H)-one with 3-pentanone afforded the cis-5,6-dihydro-7H-pyrrolo[3,2-f]quinolin-2(1H)-one. Oxidation with DDQ in CH2Cl2 gave 6-ethyl-5-methyl-7-(2,2,2-trifluoroethyl)-4-trifluoromethyl-1H-pyrrolo[3,2-f]quinolin-2(1H)-one (IX). The latter exhibited 76% androgen receptor agonist efficacy with a potency (EC50) of 7.6 nM relative to dihydrotestosterone in co-transfection assays using CV-1 cells and displayed androgen receptor binding activity (IC50) of 1.7 nM. Pharmaceutical compns. and formulations of IX are also disclosed. I-VIII are useful for the treatment of acne, male-pattern baldness, impotence, sexual dysfunction, wasting disease, hirsutism, hypogonadism, prostatic hyperplasia, osteoporosis, cancer cachexia, and hormone-dependent cancers (no data). Pharmaceutical compns. and formulations of IX are also disclosed.

IT 453592-26-2P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical

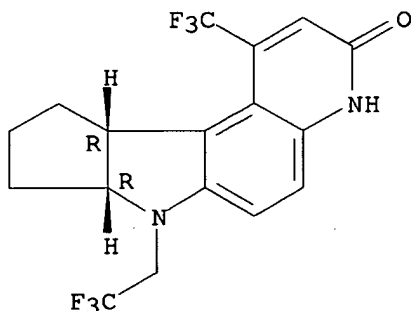
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process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses) (androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-26-2 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 453592-85-3P 453592-86-4P

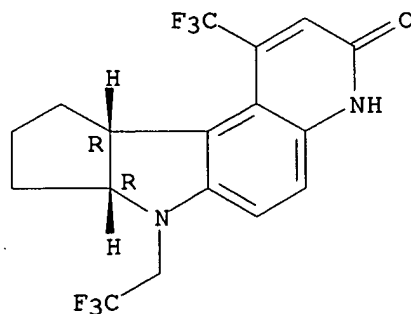
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-85-3 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

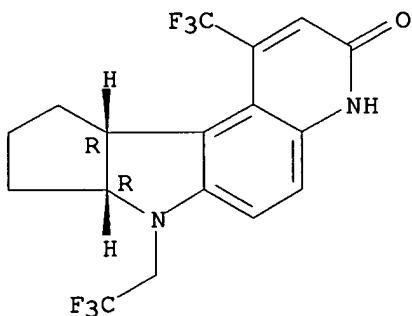


RN 453592-86-4 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(-)- (9CI) (CA INDEX NAME)

10080926

Rotation (-). Absolute stereochemistry unknown.

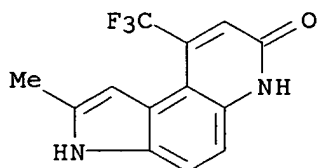


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453592-47-7P 453592-52-4P 453592-53-5P
453592-54-6P 453592-57-9P 453592-60-4P
453592-71-7P 453592-72-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

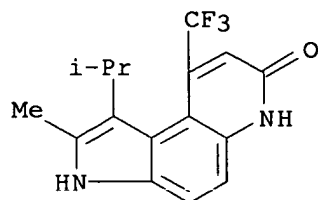
RN 453592-19-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)-
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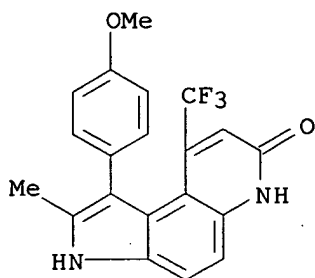
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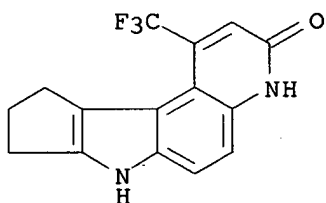
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



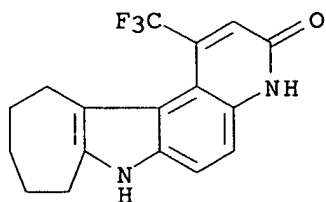
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CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-25-1 CAPLUS

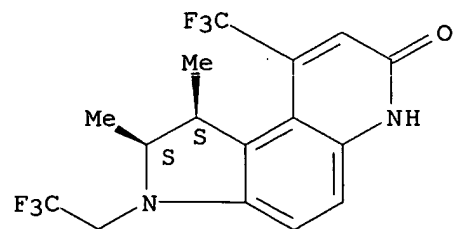
CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10,11,12-hexahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-30-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

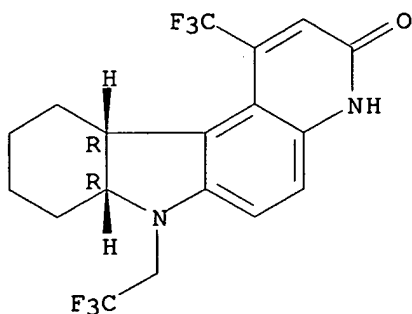


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RN 453592-39-7 CAPLUS

CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7,7a,8,9,10,11,11a-octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,11aR)-rel- (9CI) (CA INDEX NAME)

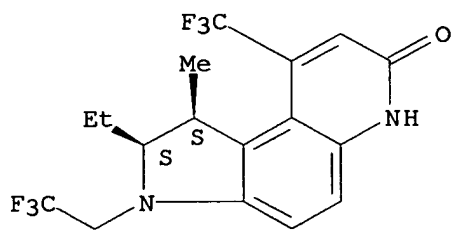
Relative stereochemistry.



RN 453592-41-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-1,2,3,6-tetrahydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

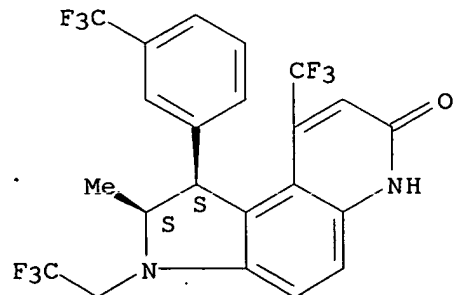
Relative stereochemistry.



RN 453592-46-6 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

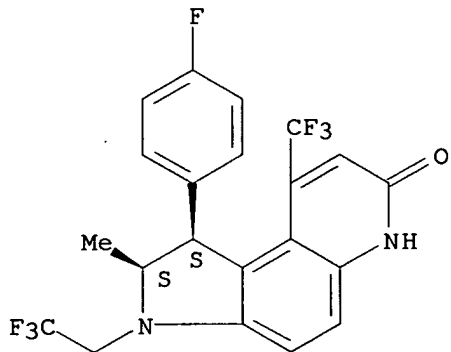


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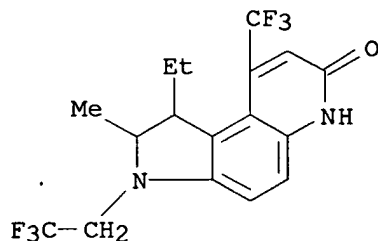
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



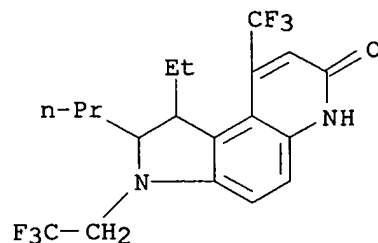
RN 453592-52-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-53-5 CAPLUS

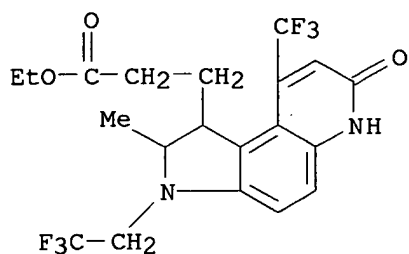
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-54-6 CAPLUS

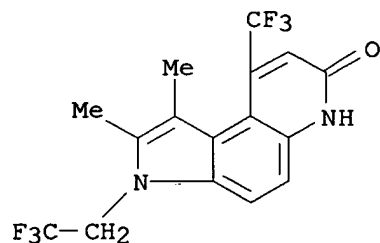
CN 1H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 2,3,6,7-tetrahydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

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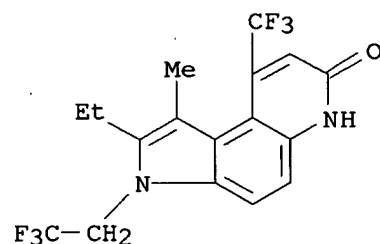
RN 453592-57-9 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-60-4 CAPLUS

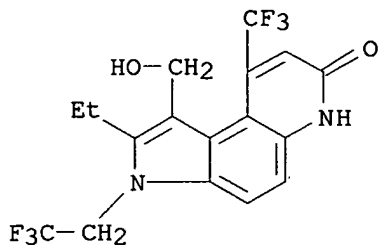
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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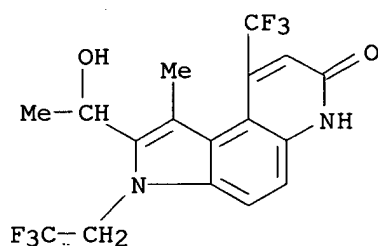
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-(hydroxymethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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RN 453592-72-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-hydroxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 453592-21-7P 453592-23-9P 453592-28-4P

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453592-35-3P 453592-36-4P 453592-37-5P

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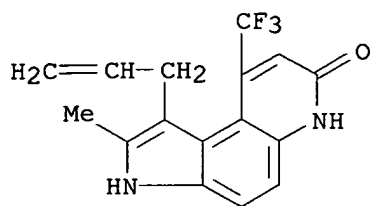
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-21-7 CAPLUS

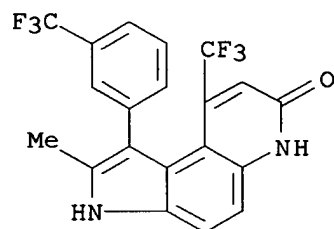
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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RN 453592-23-9 CAPLUS

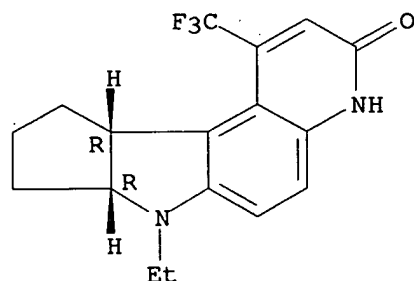
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 453592-28-4 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-ethyl-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

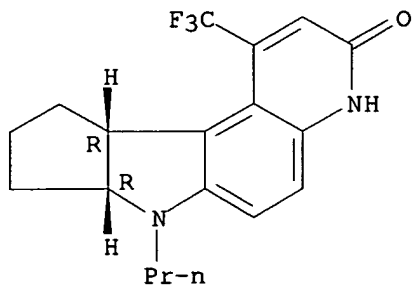


RN 453592-32-0 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-propyl-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

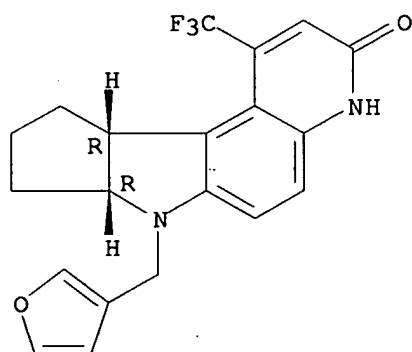
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RN 453592-33-1 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(3-furanylmethyl)-
7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA
INDEX NAME)

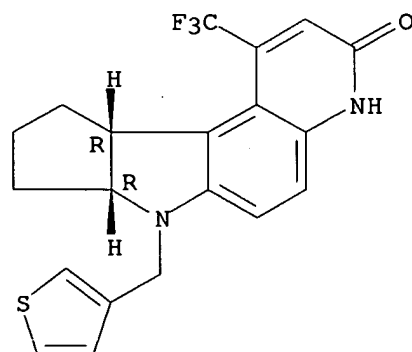
Relative stereochemistry.



RN 453592-34-2 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-
7-(3-thienylmethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX
NAME)

Relative stereochemistry.



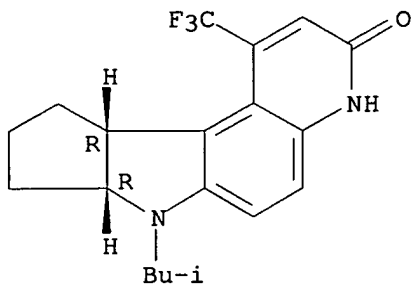
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NAME)

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NAME)

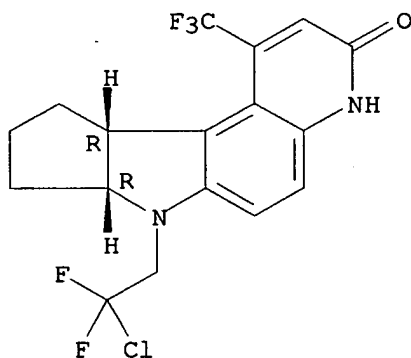
Relative stereochemistry.



RN 453592-36-4 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2-chloro-2,2-difluoroethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

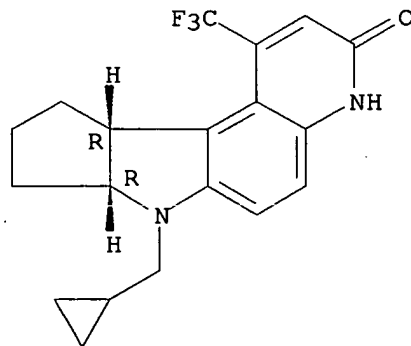
Relative stereochemistry.



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CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(cyclopropylmethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

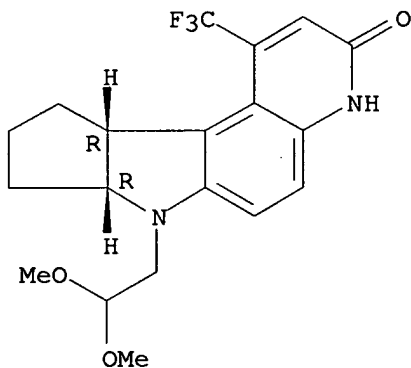


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RN 453592-38-6 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2,2-dimethoxyethyl)-
7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA
INDEX NAME)

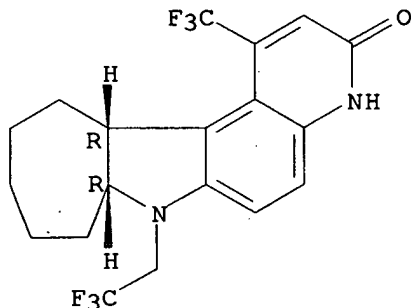
Relative stereochemistry.



RN 453592-40-0 CAPLUS

CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,11,12,12a-
octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,12aR)-rel-
(9CI) (CA INDEX NAME)

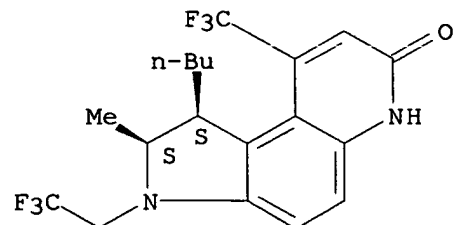
Relative stereochemistry.



RN 453592-42-2 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-butyl-1,2,3,6-tetrahydro-2-methyl-3-
(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX
NAME)

Relative stereochemistry.

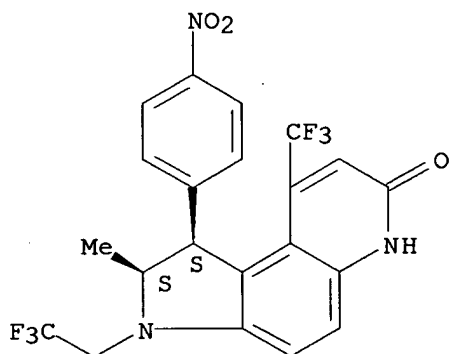


10080926

RN 453592-43-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(4-nitrophenyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

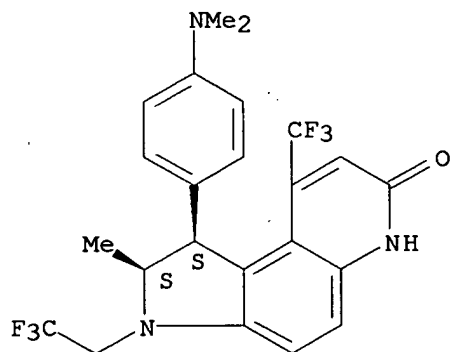
Relative stereochemistry.



RN 453592-44-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[4-(dimethylamino)phenyl]-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

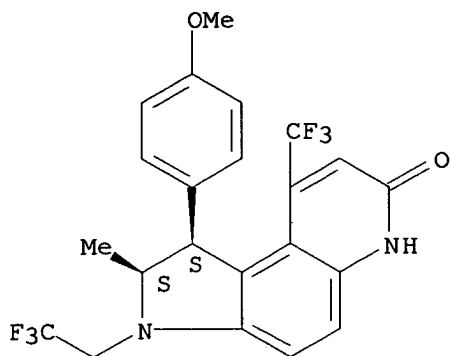


RN 453592-45-5 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

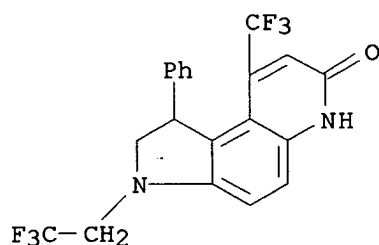
Relative stereochemistry.

10080926



RN 453592-48-8 CAPLUS

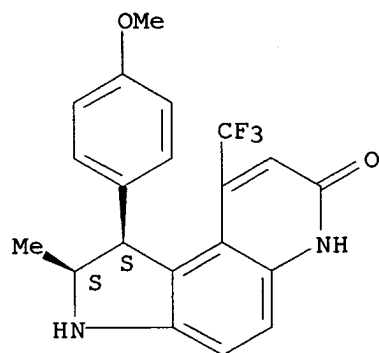
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-phenyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-49-9 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

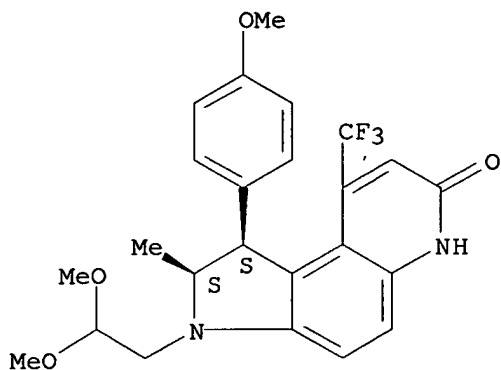


RN 453592-50-2 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-dimethoxyethyl)-1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

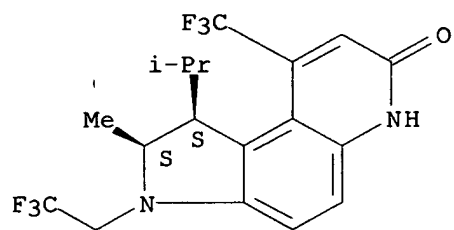
10080926



RN 453592-51-3 CAPLUS

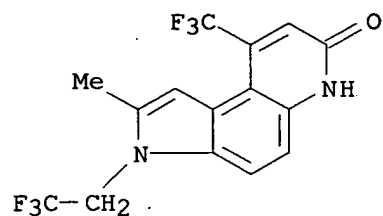
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(1-methylethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 453592-59-1 CAPLUS

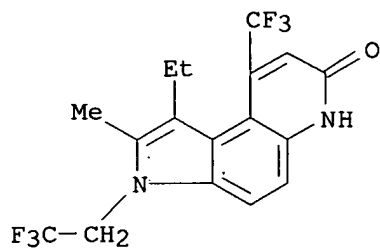
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-61-5 CAPLUS

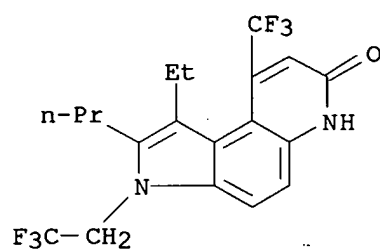
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



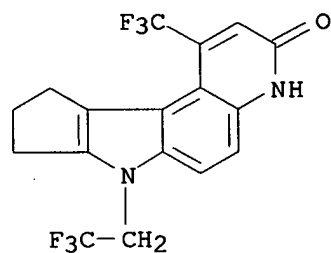
RN 453592-62-6 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



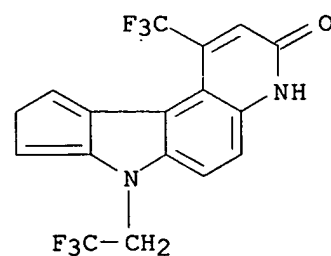
RN 453592-63-7 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-64-8 CAPLUS

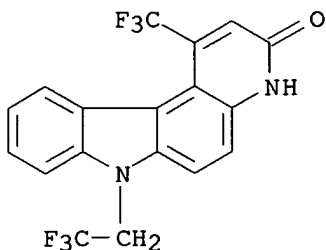
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,9-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



10080926

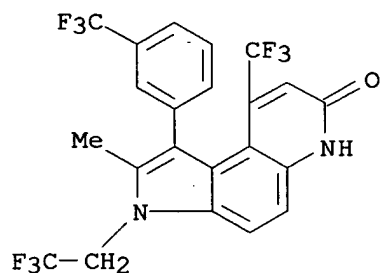
RN 453592-65-9 CAPLUS

CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



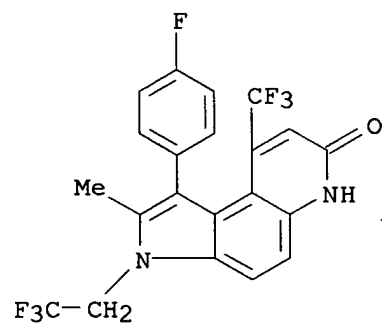
RN 453592-67-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 453592-68-2 CAPLUS

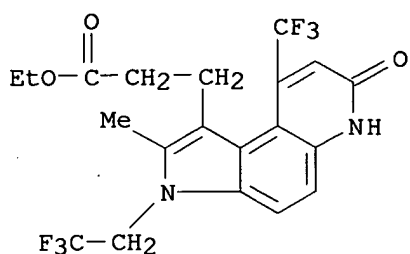
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-69-3 CAPLUS

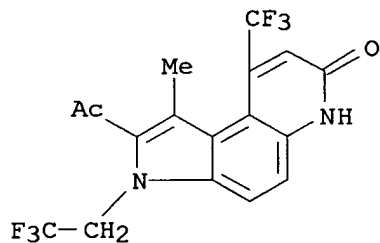
CN 3H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

10080926



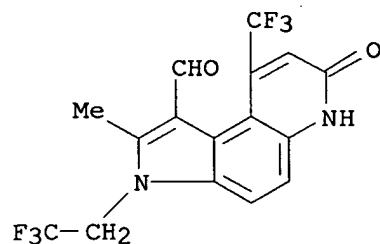
RN 453592-73-9 CAPLUS.

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-acetyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-74-0 CAPLUS

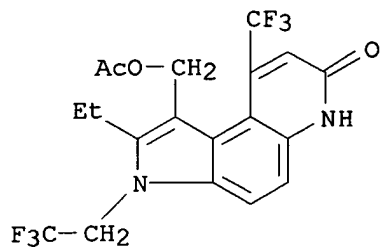
CN 3H-Pyrrolo[3,2-f]quinoline-1-carboxaldehyde, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-75-1 CAPLUS

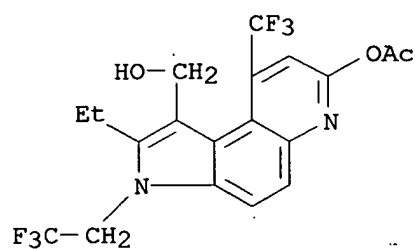
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[(acetyloxy)methyl]-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



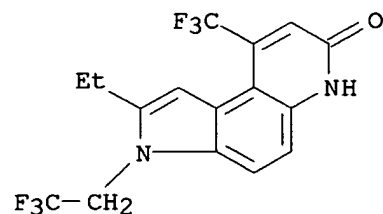
RN 453592-76-2 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinoline-1-methanol, 7-(acetyloxy)-2-ethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



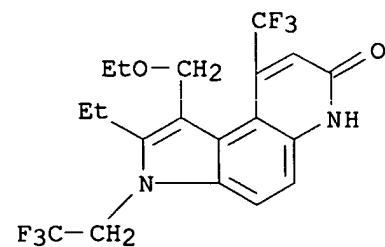
RN 453592-77-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-78-4 CAPLUS

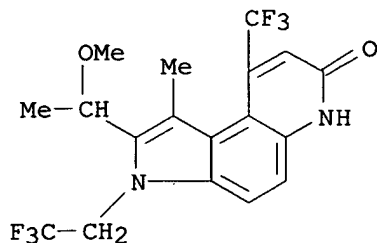
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(ethoxymethyl)-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



10080926

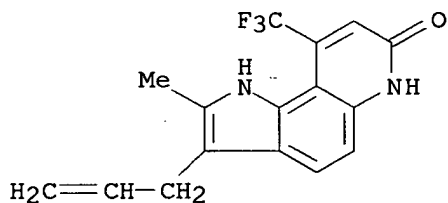
RN 453592-79-5 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-methoxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



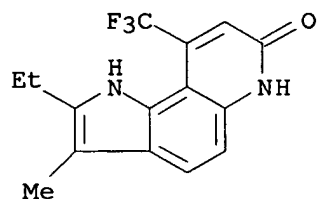
RN 453592-80-8 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-3-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-82-0 CAPLUS

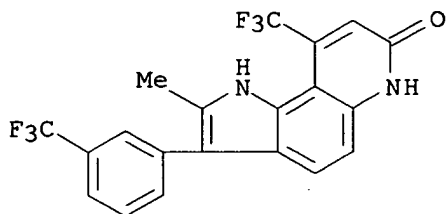
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 2-ethyl-1,6-dihydro-3-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-83-1 CAPLUS

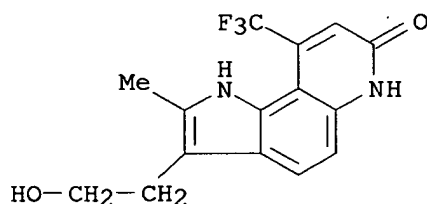
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-9-(trifluoromethyl)-3-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

10080926



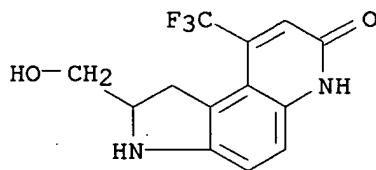
RN 453592-84-2 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-3-(2-hydroxyethyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



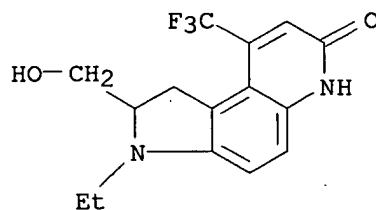
RN 453593-25-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453593-26-5 CAPLUS

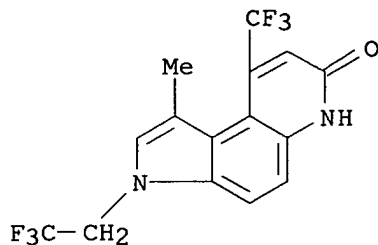
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-ethyl-1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453593-30-1 CAPLUS

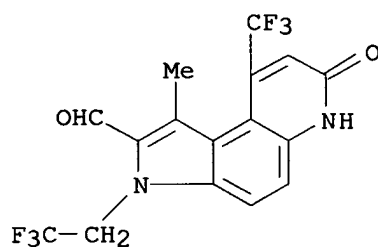
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



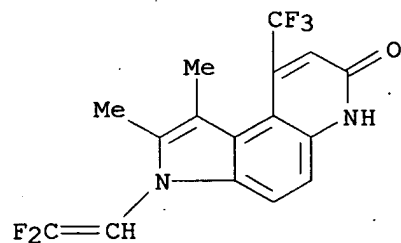
RN 453593-31-2 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinoline-2-carboxaldehyde, 6,7-dihydro-1-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453593-32-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-difluoroethenyl)-3,6-dihydro-1,2-dimethyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:455695 CAPLUS

DN 131:213835

TI Reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines

AU Yamashkin, S. A.; Trushkov, I. V.; Tomilin, O. B.; Terekhin, I. I.; Yurovskaya, M. A.

CS Mordovian State Pedagogical Institute, Sarinsk, 430007, Russia

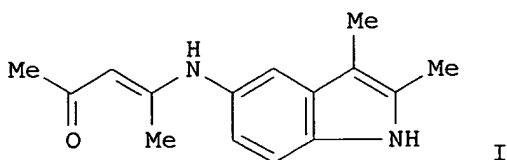
SO Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), Volume Date 1998, 34(9), 1050-1065

CODEN: CHCCAL; ISSN: 0009-3122

PB Consultants Bureau

10080926

DT Journal
LA English
GI



AB The concept of regioorientation is proposed for the annelation of the pyridine ring with the participation of 5-, 6-, and 7-aminoindoles (e.g., I). The conclusions based on the exptl. data are supported by semiempirical AM1, PM3, and MNDO quantum-chemical calcs.

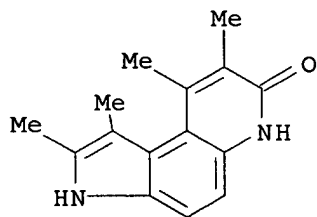
IT 243669-00-3 243669-02-5 243669-06-9

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of pyrroloquinolines)

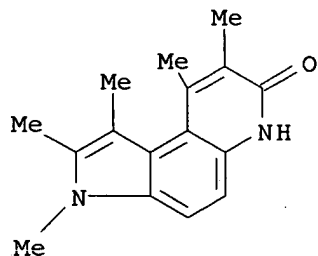
RN 243669-00-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,8,9-tetramethyl- (9CI)
(CA INDEX NAME)



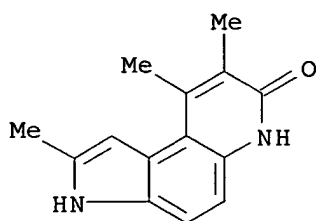
RN 243669-02-5 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,3,8,9-pentamethyl- (9CI)
(CA INDEX NAME)



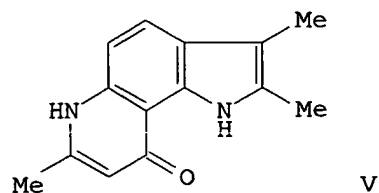
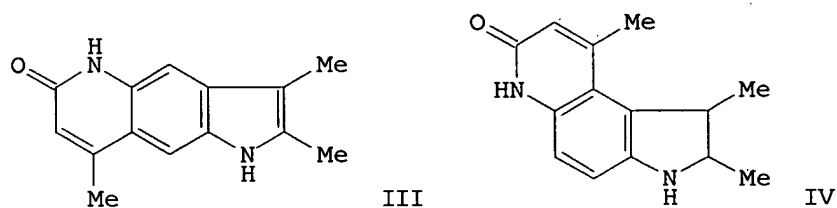
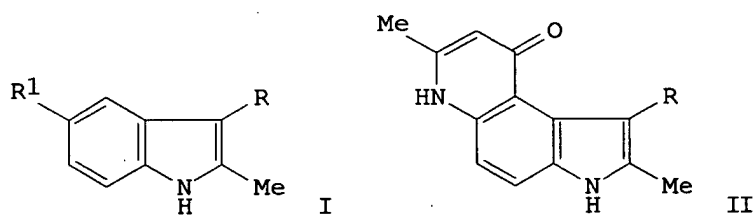
RN 243669-06-9 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2,8,9-trimethyl- (9CI) (CA INDEX NAME)



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:438395 CAPLUS
DN 99:38395
TI Synthesis of pyrroloquinolones
AU Yamashkin, S. A.; Yudin, L. G.; Kost, A. N.
CS Mosk. Gos. Univ., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1983), (4), 493-7
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
OS CASREACT 99:38395
GI



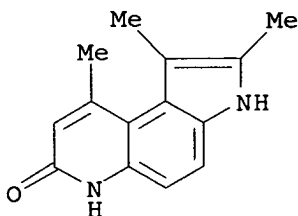
10080926

AB Intramol. cyclocondensation of I (R = Me, H; R1 = EtO2CCH:CMenH) by refluxing in biphenyl gave 89 and 95% pyrroloquinolines II. Similarly, refluxing I (R = Me, R1 = MeCOCH2CONH) in F3CCO2H gave a mixture containing III and IV. Refluxing I (R = Me, R1 = EtO2CCH:CMenH in the 6 position) with biphenyl gave 90% V.

IT **86269-88-7P 86269-91-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

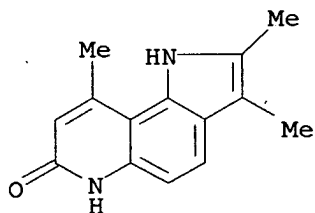
RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA INDEX NAME)



RN 86269-91-2 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2,3,9-trimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1948:32006 CAPLUS

DN 42:32006

OREF 42:6783h-i,6784a-i,6785a-i,6786a-i,6787a-i,6788a-e

TI Orienting experiments on the reaction mechanism of aromatic bicyclic compounds

AU Huisgen, Rolf

CS Univ. Munich, Weilheim, Germany

SO Ann. (1948), 559, 101-52

DT Journal

LA Unavailable

OS CASREACT 42:32006

GI For diagram(s), see printed CA Issue.

AB A comprehensive monograph dealing largely with the theory of the reaction mechanism of naphthalene (I) and divided into the following parts: 1) static fixation of the double bonds in I; 2) fusion of a 3rd ring to derivs. of I; 3) structure of the I nucleus and the manner in which it reacts; 4) anellation and excitation structures in the I series; 5) naphthalenoid and benzenoid bicyclic compds.; 6) manner in which quinoline

(II) and 1-hydroxyquinoline (III) react; 7) reactivity of aromatic polycyclic compds. (much of which involves the critical evaluation of previous work); and 8) an extensive exptl. part. The reactions of bicyclic compds. are discussed at length in terms of quantum-mech. calcns. of resonance energies (cf. Pauling and Wheland, C.A. 27, 3877; Sherman, C.A. 28, 6631.3; and Penney, C.A. 31, 2513.2). The hypothesis formulated by Marckwald (Ber. 23, 1015 (1890)) that the double bonds in I remain fixed loses its significance when anellation reactions (involving a 3rd ring) are considered. Previously the assumption was made that an "angular" tricyclic compound (IV) was normally formed. This was shown to be true in the case of 1-bromo- or 1-nitro-2-naphthylamine, either of which lose the 1-substituent on further cyclization to form the angular benzoquinoline. However, H. has shown that under certain conditions, a linear tricyclic form (V) may result. When 2 g. 1,2-MeC10H6NHAc (VI), m. 193°, was refluxed gently 5 hrs. with 2 g. arsenious acid, 7 g. glycerol, 7 g. H2SO4, and 5 g. AcOH, followed by treatment with 15 cc. H2O, digestion with NH4OH-CHCl3, filtration, evaporation of the CHCl3 extract, digestion with 8 g. Ac2O, saturation with NH4OH, reextn. with CHCl3, and treatment with 2 N HCl, H. obtained (after removal of residual VI, retreatment with NH4OH-CHCl3, and filtration through Al2O3) 0.53 g. 8-methyl-6,7-benzoquinoline (VII), b12 200°, m. 53-4° (not recrystd. due to high solubility in organic solvents); picrate, triclinic orange prisms (from MeOH), m. 212° (decomposition). The mother liquors gave no trace of the known "angular" 5,6-benzoquinoline (VIII) (picrate, m. 254°). The HCl salt (IX) of VII forms golden yellow needles. The yellow perchlorate and orange-red nitrate of VII contrast sharply with the corresponding colorless salts of VIII. In ultraviolet light, VII in Me2CO shows intense light blue, and IX a pale yellow fluorescence. On the other hand, VIII in organic solvents shows a very slight blue and its HCl salt gives a stronger blue fluorescence. 1,2-MeC10H6NHCOCH2Ac (cf. Limpach, C.A. 25, 3999), m. 135°, (0.25 g.) was shaken with 2.5 cc. concentrated H2SO4, allowed to stand 1 hr., poured into ice-H2O, made alkaline with NH4OH, extracted with CHCl3, evaporated, and taken up in MeOH, yielding 0.16 g. 2-hydroxy-4,8-dimethyl-6,7-benzoquinoline, pale yellow (sublimable) needles, m. 253°, insol. in aqueous alkaline solns. and in aqueous acids, but soluble in concentrated H2SO4 with a yellow color and yellowish green fluorescence, and giving a blue-green ultraviolet fluorescence in MeOH. On the other hand the "angular" 4-methyl-5,6-benzocarbostyryl shows practically no ultraviolet fluorescence in MeOH and a deep violet fluorescence in H2SO4. Very similarly 0.35 g. 1,2-BrC10H6NHCOCH2Ac, m. 117°, in H2SO4 was cyclized to 0.225 g. 2-hydroxy-4-methyl-8-bromo-6,7-benzoquinoline, pale yellow needles, m. 232-4°. From 2 g. 1,2-MeC10H6NH2 and 1.6 g. AcCH2CO2Et, H. obtained 2.5 g. 1-MeC10H6NHCMe:CHCO2Et, m. 86-7° (from MeOH), 1.5 g. of which, gradually added to 20 g. paraffin oil at 270°, followed by heating 10 min. at 280°, gave 0.85 g. "linear" 2,8-dimethyl-4-hydroxy-6,7-benzoquinoline, yellow needles, m. 340° (decomposition) (after successive crystns. from C6H6, PhNO2, and EtOH), very soluble in 2 N NaOH, slightly soluble in hot 2 N HCl, showing marked blue-green ultraviolet fluorescence in NaOH, blue in NaOH, and yellowish green in concentrated H2SO4. From 0.3 g. 2-C10H7NHNH2.HCl in 4 cc. MeOH with 0.2 cc. cyclohexanone, H. obtained a nearly quant. yield of 5,6-benzo-1,2,3,4-tetrahydrocarbazole (X), m. 137° (from MeOH); dark brown picrate, m. 192° (from C6H6). The formation of X is expedited by adding 2 N HCl to the original reaction mixture 1,2-MeC10H6NHAc, m. 193°, was hydrolyzed with HCl in alc. and 3.5 g. of the resulting salt in 25 cc. 7 N HCl was treated at 0° in 8 cc. H2O with 1.34 g. NaNO2, followed by treatment with urea and addition to

12 g. SnCl_2 in 8 cc. HCl and 110 cc. H_2O , giving a nearly quant. yield of 1-methyl-2-hydrazinonaphthalene- HCl (XI), leaflets (from HCl), m. 195° (decomposition), converted by AcONa into the free base, m. 110° (from MeOH), reducing Fehling solution XI with Me_2CO gave 2,1-Me $2\text{C}:\text{NNHC10H6Me}$, leaflets, m. 99° . By heating 0.85 g. XI in 2 cc. AcOH with 1 cc. cyclohexanone and 20 mg. NiCl_2 2 hrs. at 180° , and then 3 hrs. at 200° , a small amount of X was obtained, showing that ring closure had removed the 1-Me group. Careful warming of 135g. 3,6-(H_2N)(O_2N) $\text{C}_6\text{H}_3\text{Me}$ with 125 g. arsenic acid, 270 g. glycerol, and 250 g. H_2SO_4 about 6 hrs. gave 108 g. of a difficultly separated mixture of 6-nitro-7-methylquinoline (XII) and its 5-Me isomer (XIII), from which 11.4 g. XIII, m. 165° (colorless HCl salt), was separated by successive crystns. from MeOH and Me_2CO . Inasmuch as the components in the mother liquors from XIII could not be fractionally crystallized, the solution was evaporated,

treated with 350 cc. MeOH , and shaken 40 min. with 180 cc. hot 20% KOH in MeOH , followed by the addition of 700 cc. MeOH , yielding a highly insol. conversion product of XIII, the filtrate and washings from which gave 54 g. pure XII, colorless needles (from EtOH), m. 140° ; colorless HCl salt. SnCl_2 reduction of XIII yielded 6-amino-5-methylquinoline, coarse prisms, m. $163-4^\circ$ (from C_6H_6) (yellow HCl salt; Ac derivative m. 168°), which when diazotized and poured into a Cu_2O suspension in EtOH gave 5-methylquinoline, pale yellow oil (picrate m. $213-14^\circ$) (cf. Skraup and Brunner, Monatsh. 7, 141(1886)), 0.43 g. of which after treatment 10 hrs. with 0.65 g. CrO_3 and 5 cc. 35% H_2SO_4 gave 5-carboxyquinoline, m. 330° (cf. Yakubovich, C.A.5,503). By a similar series of reactions XII gave the following: 6-amino-7-methylquinoline, plates, m. 139° (from C_6H_6); 7-methylquinoline (picrate, m. 235° , identical with that prepared from 3-Me $\text{C}_6\text{H}_4\text{NH}_2$ by the Skraup synthesis); 7-carboxyquinoline, m. 245° . XIII (1 g.) heated at the b.p. 3 min. with 12 cc. 10% KOH in MeOH gave 0.79 g. 1,2-bis(6-nitro-5-quinolyl)ethane, m. 300° (decomposition) (from AcOH), also formed when 2 N NaOH or alkaline arsenite solns. are used in place of KOH . The corresponding diamine, $\text{C}_{20}\text{H}_{18}\text{N}_4$, formed greenish yellow needles (from C_6H_6) (properties not given). By analogous procedures H. obtained from 6-nitro-5,8-dimethylquinoline 1,2-bis(6-nitro-8-methyl-5-quinolyl)ethane, nearly colorless needles, m. 257° (from pyridine or AcOH), and from 5-nitro-8-methylquinoline 1,2-bis(5-nitro-8-quinolyl)ethane, needles, m. 221° (from C_6H_6 or AcOH), which on further treatment with alkali gave a deep violet color (cf. Trautmann, Ber. 23, 3673(1890)). 2- $\text{O}_2\text{NC}_6\text{H}_4\text{Me}$ in cooled absolute Et_2O , treated with an equimol. amount of alc.-free EtOK in Et_2O , the mixture let stand overnight, shaken with H_2O , and the Et_2O layer dried, filtered through Al_2O_3 , and concentrated, gave 25-30% o,o'-dinitrobibenzyl, needles (from MeOH), m. 122° . Knuppel's reaction (cf. Ann. 310, 75(1900)), in which 6-nitroquinoline was heated with MeONa , gave 80% of a quinazone N-oxide (XIV), yellow needles, decomposing 330° (from AcOH) (red HCl salt (from H_2O)), which when distilled with Fe powder gave the O-free quinazone, $\text{C}_{18}\text{H}_{10}\text{N}_4$, pale yellow leaflets (from C_6H_6), m. 369° , sublimes undecompd. at 400° , gives a colorless HCl solution, and when heated with Zn dust, yields a bluish green semiquinone-like compound that may be reoxidized to the original quinazone by KMnO_4 . A reaction analogous to that giving XIV yielded from XII the 7,7'-di-Me derivative, yellow needles (from AcOH), m. 355° (decomposition), yielding, on reduction, the dimethylquinazone, $\text{C}_{20}\text{H}_{14}\text{N}_4$, long, pale yellow needles, m. 380° (from xylene). Similarly 6-nitro-7,8-dimethylquinoline gave the corresponding tetra-Me derivative of XIV, yellowish green needles (from PhNO_2), decomposing above 330° and forming, when distilled with Fe , the tetramethylquinazone, pale yellow needles, m. 354° . 6-Nitroquinoline (1 g.), 0.5 g. KCN , 15 cc. EtOH , 3 cc. H_2O , and 0.5 g.

KOH heated 4 hrs. gave 0.5 g. 5-cyano-6-ethoxyquinoline, needles, m. 130° (from MeOH), very resistant to HNO₂, hot concentrated HCl, and cold H₂SO₄, whose colorless HCl and H₂SO₄ salts are difficultly soluble in H₂O. By a similar reaction, using MeOH in place of EtOH, 5-cyano-6-methoxyquinoline, needles (from MeOH), m. 179°, was obtained. To a cooled mixture of 5 g. 6-nitroquinoline, 6 g. HONH₂.HCl, and 90 cc. EtOH was added (in 1 portion) 30 cc. 20% KOH in MeOH. The exothermic reaction gave rise to 94% 5-amino-6-nitroquinoline (XV), yellow needles, m. 272° (yellow, difficultly soluble HCl salt), which with SnCl₂ in HCl gave 5,6-diaminoquinoline chlorostannate; the latter, after detinning with H₂S, yielded the HCl salt, pale yellow crystals, 0.1 g. of which when heated with 0.12 g. benzil in 5 cc. alc. and small amts. of AcONa gave the substituted quinoxaline, C₂₃H₁₅N₃ (0.88 g.), plates from C₆H₆, m. 205°; the di-Ac derivative m. 252° with decomposition to form 5,6-(methylimidazolo)quinoline, m. 200° (hydrate, m. 70°). The latter was more readily prepared by heating 0.5 g. XV in 5 cc. AcOH several hrs. with 2.1 g. SnCl₂ in 4 cc. HCl, followed by detinning, evaporation, treatment with NH₄OH, and extraction with Me₂CO. Similarly, when

XV

was reduced in the presence of HCO₂H (instead of AcOH), 5,6-imidazoloquinoline, m. 214° (from C₆H₆) (hydrate, m. 78°), was formed. By diazotization, the NH₂ group in XV was replaced by iodine (using KI and Cu-bronze), yielding a resin which after trituration with HCl, extraction with NH₄OH·CHCl₃, followed by washing with aqueous

Na₂SO₄ and H₂O, and passing the CHCl₃ solution through Al₂O₃, gave red needles, which on repeated crystallization from MeOH and C₆H₆ yielded colorless 5-iodo-6-chloroquinoline, m. 136°. Deiodination with Cu-bronze in boiling PhNO₂ gave 6,6'-dichloro-5,5'-biquinoline, colorless polyhedrons, m. 205°. When, however, the iodine was removed by means of HI in AcOH, 5-iodo-6-chloroquinoline gave 6-chloroquinoline, m. 40-1°. Skraub's cyclization of 0.5 g. 5-nitro-6-aminoquinoline (Kaufmann and Zeller, C.A. 12, 1390), using arsenic acid gave 0.115 g. 4,7-phenanthroline, polyhedrons (from C₆H₆), m. 174° (showing only a faint ultraviolet fluorescence), also obtained (in 65% yield) by cyclization of 5-bromo-6-aminoquinoline. Evidently NO₂ or Br in position 5 fails to block the formation of 4,7-phenanthroline. On the other hand, when 1 g. 6-acetamido-5-methylquinoline was heated gently 10-12 hrs. with 0.9 g. arsenic acid, 6 g. glycerol, 6 g. H₂SO₄, and 5 g. glacial AcOH, followed successively by treatment with H₂O, extraction with NH₄OH·CHCl₃,

extraction

with 2 N HCl, reextn. with NH₄OH·CHCl₃, evaporation, treatment of the dry extract

with 3 cc. pyridine and 0.2 g. 4-MeC₆H₄SO₂Cl (to remove any unchanged starting product), and continued purification by extracting alternately with alkaline CHCl₃ and HCl, filtering the CHCl₃ solution through Al₂O₃, and finally subjecting the product to microdistn., using a water pump, H. obtained 3 fractions: (a) subliming 180°, (b) yellow oil, b. 200-20°, and (c) a red oil, b. 235°. Of these (b) gave 12 mg. linear 10-methyl-1,5-anthrazoline hydrate, C₁₅H₁₀N₂·3H₂O, felted needles, m. 62°, giving a yellow solution in acids and showing a brilliant bluish violet (ultraviolet) fluorescence. 8-Methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline (XVI), m. 225-6° (from EtOH), was prepared in 70% yield by heating 0.5 g. 6-hydrazino-8-methylquinoline (the synthesis of which is not given) with 3 cc. AcOH and 1.5 cc. cyclohexanone 6 hrs. and purifying the product by methods similar to those given above. XVI was also readily obtained in 75% yield by heating 0.33 g. of the substituted cyclohexanone hydrazone (XVII), m. 189°, at 200-240° with 15 mg. dry NiCl₂, or (in only 34% yield) by heating this same hydrazone with 2 N H₂SO₄. The following steps also led to the formation of XVI:

4-nitro-2,5-xylylidine → Skraup's synthesis 50% 6-nitro-5,8-dimethylquinoline, m. 118° (from alc.) → SnCl₂ 6-amino derivative, b₁₂ 194°, prisms, m. 175° → HCl salt, yellow → 7 N HCl+HNO₂ diazo derivative → SnCl₂ chlorostannate → H₂S+HCl 85% 6-hydrazino-5,8-dimethylquinoline-HCl, yellow needles (free base (XVIII), m. 185°) → cyclohexanone 30% XVI. The ultraviolet absorption spectra of XVI prepared by the various methods were identical and showed a striking similarity to that of 7,8-dimethyl-10,11-tetramethylene-5,6(N)-pyrroquinoline. XVIII fails to undergo cyclization to XVI unless HCl is present. 6-Hydrazino-8-methylquinoline-HCl and MeCOEt in AcOH gave 40% 8,10,11-trimethyl-5,6(N)-pyrroquinoline, m. 188° (from EtOH), also formed in poor yield from the HCl salt of XVIII with concomitant removal of a Me group. Similarly, 0.5 g. 5-hydrazinoquinoline-HCl and cyclohexanone in AcOH gave 0.42 g. 10,11-tetramethylene-5(N),6-pyrroquinoline (XIX), m. 289° (from Me₂CO). XIX was also isolated in 1-2% yield after extensive purification from 5-hydrazino-6-methylquinoline, m. 158° (pale yellow HCl salt).

SnCl₂ reduction of 15 g. 6-nitro-2-hydroxylepidine gave 9.6 g. 2-hydroxy-4-methyl-6-aminoquinoline (XX), pale yellow, m. above 300°, cyclizing in the presence of arsenic acid, glycerol, and H₂SO₄-AcOH, followed by successive treatments with HCl and NH₄OH, to form 2-hydroxy-4-methyl-4,7-phenanthroline (XXI), colorless prisms, the "angularity" of which was attested to by its very faint ultraviolet fluorescence, its ready solubility in aqueous NaOH and in boiling aqueous Na₂CO₃, and

by the fact that its salts are colorless. 2,5-Xylylidine, when heated at 160° with an equimol. amount of AcCH₂CO₂Et, gave the N-acetylacetyl derivative, m. 96° (from aqueous MeOH), which when heated 0.5 hr. on a steam bath with 6 parts concentrated H₂SO₄ gave (after pouring on ice) 90% 2-hydroxy-4,5,8-trimethylquinoline, m. 238° (from EtOH); 6-nitro derivative, pale yellow, m. 275° (from AcOH or EtOH); 6-amino derivative (XXII) (formed from the orange-red Sn double salt), pale yellow leaflets, m. 302° (from aqueous NH₄OH or EtOH) (colorless HCl salt, difficultly soluble in H₂O). The Skraup cyclization of XXII gave 2-hydroxy-4,9,10-trimethyl-1,5-anthrazoline (XXIII), pale yellow needles (from glacial AcOH or Ac₂O), m. 290°, whose linear structure was indicated by the yellow color of its acid solns., its insoly. in alkali, and its strong blue ultraviolet fluorescence in MeOH. On diazotization, followed by SnCl₂ reduction, XX gave 90% 2-hydroxy-4-methyl-6-hydrazinoquinoline, colorless needles from H₂O, decomposing 240°, reducing Fehling solution in the cold, and forming a colorless HCl salt, which, when cyclized in the presence of MeCOEt and glacial AcOH, gave 90% 2-hydroxy-4,10,11-trimethyl-5,6(N)-pyrroquinoline, needles (from alc.), m. above 300° (decomposition); yellow HCl salt. When an analogous cyclization was carried out in the presence of cyclohexanone, 2-hydroxy-4-methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline, m. above 300°, was formed; golden yellow HCl salt. Diazotization of XXII, followed by reduction, gave the yellow chlorostannate of 2-hydroxy-4,5,8-trimethyl-6-hydrazinoquinoline, which in hot H₂O, followed by filtration of the stannic acid, reacted with MeCOEt to form the corresponding substituted hydrazone, pale yellow needles, m. 112° (from a buffered AcONa solution), which failed to cyclize when treated with ZnCl₂ at 200-60°, giving only 4,5,8-trimethylcarbostyril, m. 236°. Other attempts to cyclize the compound were equally unsuccessful. 2,3-Diphenyl-4,5-benzoinidole, colorless prisms with blue-green iridescence, m. 166-7°, (3 g.) was formed from 1 g. 2-H₂NC₁₀H₇, 0.5 g. C₁₀H₇NH₂.HCl, and 2.2 g. benzoin at 140-65° (cf. Japp and Murray, J. Chemical Society 65, 889(1894)). 2,1-H₂NC₁₀H₆Me subjected to a similar reaction gave 1-methyl-2-desylaminonaphthalene, 2,1-[PhC(OH):CPhNH]C₁₀H₆Me, pale yellow, m. 152-3° (from CHCl₃-MeOH),

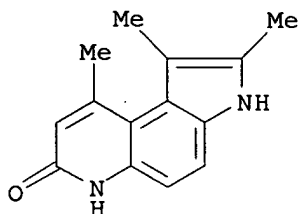
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which could not be cyclized by the use of ZnCl_2 , H_2SO_4 , H_3PO_4 , SnCl_4 , NiCl_2 , or SOCl_2 . The structure of this compound was shown by HClMeOH hydrolysis to benzoin and 2,1- $\text{H}_2\text{NC}_{10}\text{H}_6\text{Me}$. The resonance energy of I was calculated from the total hydrogenation to decahydronaphthalene and also from its partial hydrogenation to tetrahydronaphthalene. The values obtained were, resp., 63.5 and 63.1 kcal./mol. and the approx. resonance energy per ring was 31.5 kcal. (cf. also Pauling, "Nature of the Chemical Bond," C.A. 33, 6700.4).

IT **86269-88-7**, 3H-Pyrrolo[3,2-f]quinolin-7-ol, 1,2,9-trimethyl-
(preparation of)

RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA
INDEX NAME)



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(FILE 'HOME' ENTERED AT 16:05:03 ON 12 APR 2005)

FILE 'REGISTRY' ENTERED AT 16:05:13 ON 12 APR 2005

L1 STRUCTURE UPLOADED

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L3 71 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:06:04 ON 12 APR 2005

L4 5 S L3

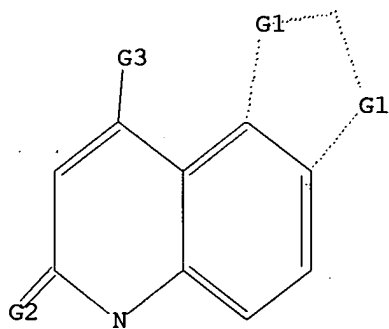
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L1 HAS NO ANSWERS

L1 STR



G1 C,N

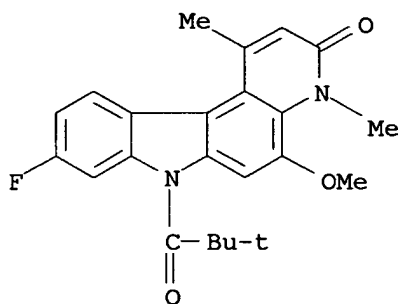
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G3 C,O,S,N,X

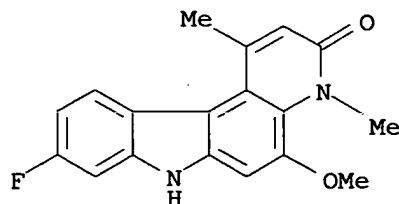
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=> d bib abs hitstr 1-5

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:39690 CAPLUS
DN 142:240350
TI An efficient procedure for the deprotection of N-pivaloylindoles, carbazoles and β -carbolines with LDA
AU Avendano, Carmen; Sanchez, J. Domingo; Menendez, J. Carlos
CS Departamento de Quimica Organica, Farmaceutica, Facultad de Farmacia, Universidad Complutense, Madrid, 28040, Spain
SO Synlett (2005), (1), 107-110
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal
LA English
AB Treatment of variously substituted indoles with an excess of LDA at 40-45 °C led to their fast and efficient deprotection. This method was also extended to N-pivaloylcarbazoles and β -carbolines.
IT **845619-80-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indoles, carbazoles, and β -carboline via LDA-mediated deprotection of N-pivaloylindoles, -carbazoles, or - β -carboline)
RN 845619-80-9 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 7-(2,2-dimethyl-1-oxopropyl)-9-fluoro-4,7-dihydro-5-methoxy-1,4-dimethyl- (9CI) (CA INDEX NAME)



IT **845619-82-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indoles, carbazoles, and β -carboline via LDA-mediated deprotection of N-pivaloylindoles, -carbazoles, or - β -carboline)
RN 845619-82-1 CAPLUS
CN 3H-Pyrido[2,3-c]carbazol-3-one, 9-fluoro-4,7-dihydro-5-methoxy-1,4-dimethyl- (9CI) (CA INDEX NAME)



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:658121 CAPLUS
DN 137:201294
TI Preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compounds as androgen receptor modulators
IN Zhi, Lin; Van Oeveren, Cornelis Arjan; Chen, Jyun-Hung; Higuchi, Robert I.
PA Ligand Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002066475	A2	20020829	WO 2002-IB537	20020223
	WO 2002066475	A3	20030123		
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	US 2002183346	A1	20021205	US 2002-80926	20020222
	CA 2434299	AA	20020829	CA 2002-2434299	20020223
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	JP 2004524309	T2	20040812	JP 2002-565989	20020223
PRAI	US 2001-271189P	P	20010223		
	WO 2002-IB537	W	20020223		
OS	MARPAT 137:201294				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title nonsteroidal tricyclic compds. I-VIII [wherein R1 = H, halo, NO2, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl or heteroalkyl; R2 = H, halo, Me, CF3, CHF2, CH2F, CF2Cl, CN, CF2OR12, CH2OR12, OR12, SO0-2R12, NR12R13, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, or alkynyl; R3-R8 = independently H, halo, OR12, NR12R13, SO0-2R12, or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, (hetero)aryl, or arylalkyl; or R3R5 or R5R7 = a bond; or C2R4R6 or C2R6R8 = (un)substituted carbocyclic or heterocyclic ring; R9 and R10 = independently H, halo, CN, OR12, NR12R13, Cm(R12)2mOR13, SO0-2R12, NR12COR13, or (un)substituted (halo)alkyl, heteroalkyl, or arylalkyl; R11 = H, halo, CN, OR14, NR14R15, SO0-2R14, CH2R14, COR14, CO2R14, CONR13R14, or (un)substituted (halo)alkyl or heteroalkyl; R12 and R13 = independently H or (un)substituted (halo)alkyl, heteroalkyl, alkenyl, alkynyl, or (hetero)aryl; R14 = H, COR15, CO2R15, CONR15R16, or (un)substituted

(halo)alkyl, heteroalkyl, or (hetero)aryl; R15 and R16 = independently H or (un)substituted (halo)alkyl, or heteroalkyl; W = O or S; X = O, S, or NR14; Y = O, S, NR12, NOR12, or CR12R13; Z = O, S, or NR12; n = 0-2; m = 0-2; or pharmaceutically acceptable salts thereof] were prepared as modulators of androgen receptors. For example, cyclization of 6-hydrazino-4-trifluoromethylquinolin-2(1H)-one with 3-pentanone afforded the cis-5,6-dihydro-7H-pyrrolo[3,2-f]quinolin-2(1H)-one. Oxidation with DDQ in CH2Cl2 gave 6-ethyl-5-methyl-7-(2,2,2-trifluoroethyl)-4-trifluoromethyl-1H-pyrrolo[3,2-f]quinolin-2(1H)-one (IX). The latter exhibited 76% androgen receptor agonist efficacy with a potency (EC50) of 7.6 nM relative to dihydrotestosterone in co-transfection assays using CV-1 cells and displayed androgen receptor binding activity (IC50) of 1.7 nM. Pharmaceutical compns. and formulations of IX are also disclosed. I-VIII are useful for the treatment of acne, male-pattern baldness, impotence, sexual dysfunction, wasting disease, hirsutism, hypogonadism, prostatic hyperplasia, osteoporosis, cancer cachexia, and hormone-dependent cancers (no data). Pharmaceutical compns. and formulations of IX are also disclosed.

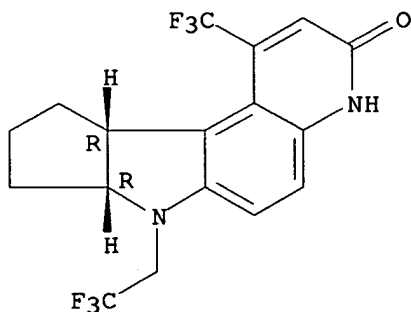
IT 453592-26-2P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses) (androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-26-2 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 453592-85-3P 453592-86-4P

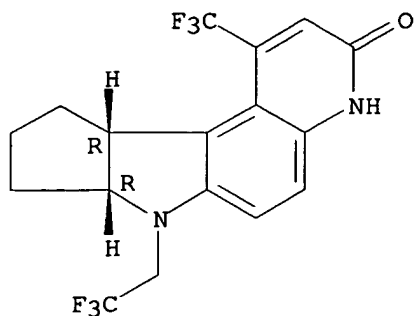
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RN 453592-85-3 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

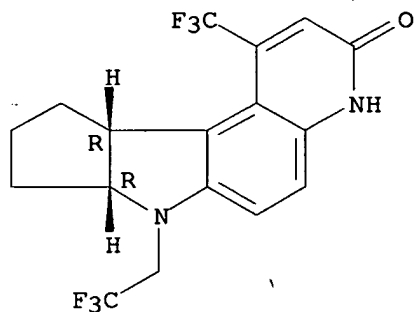
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RN 453592-86-4 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel-(-)- (9CI)
(CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



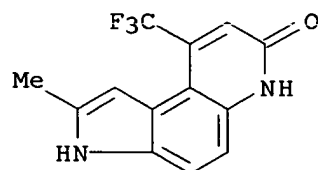
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453592-54-6P 453592-57-9P 453592-60-4P
453592-71-7P 453592-72-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

RN 453592-19-3 CAPLUS

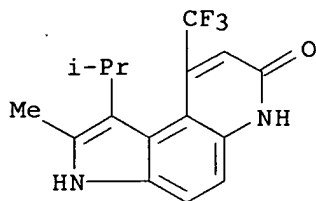
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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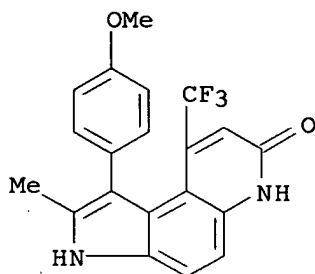
RN 453592-20-6 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(1-methylethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



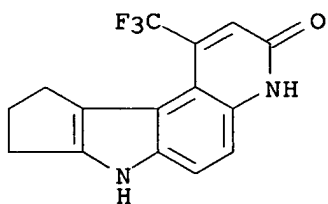
RN 453592-22-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-24-0 CAPLUS

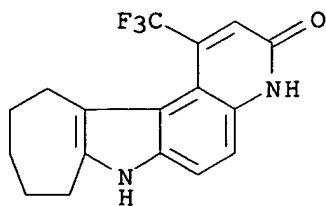
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-25-1 CAPLUS

CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10,11,12-hexahydro-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)

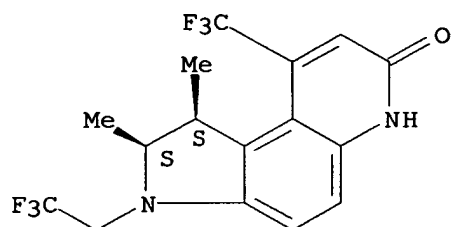
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RN 453592-30-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

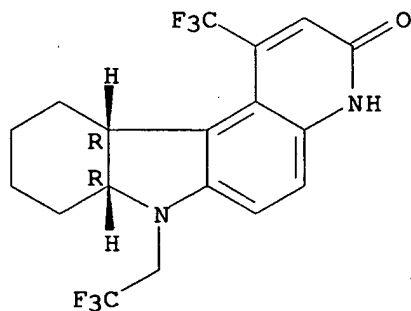
Relative stereochemistry.



RN 453592-39-7 CAPLUS

CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7,7a,8,9,10,11,11a-octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,11aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

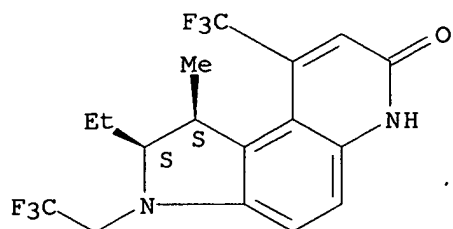


RN 453592-41-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-1,2,3,6-tetrahydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

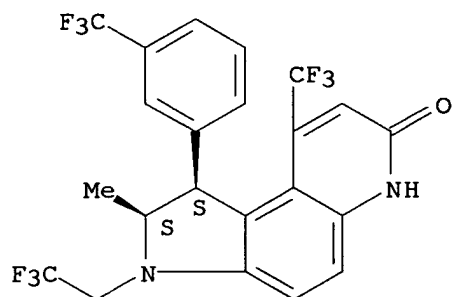
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RN 453592-46-6 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

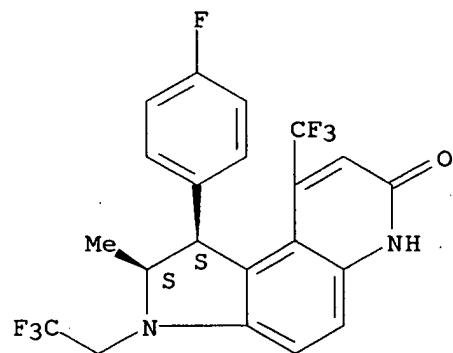
Relative stereochemistry.



RN 453592-47-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

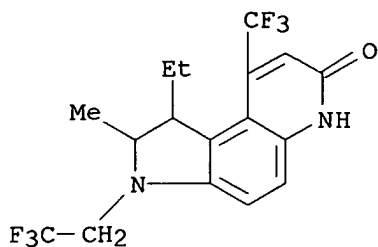
Relative stereochemistry.



RN 453592-52-4 CAPLUS

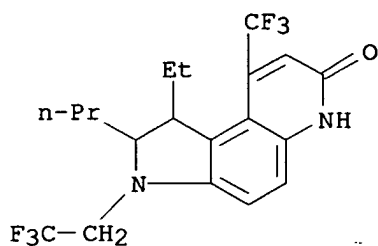
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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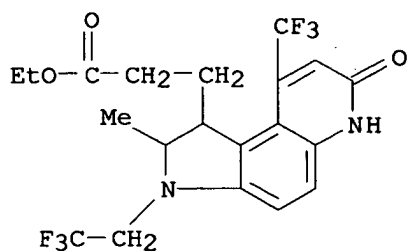
RN 453592-53-5 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-1,2,3,6-tetrahydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-54-6 CAPLUS

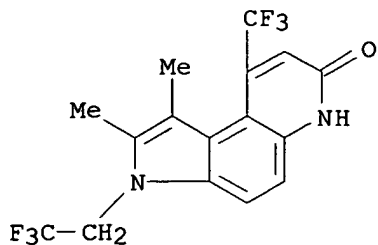
CN 1H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 2,3,6,7-tetrahydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 453592-57-9 CAPLUS

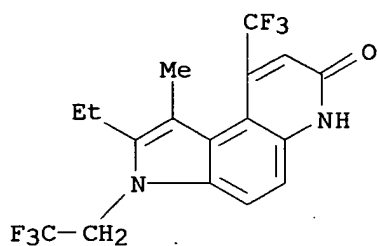
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2-dimethyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



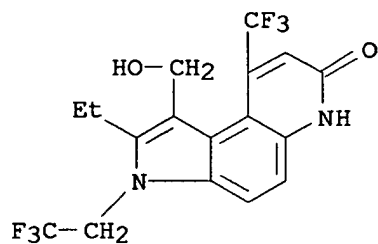
RN 453592-60-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



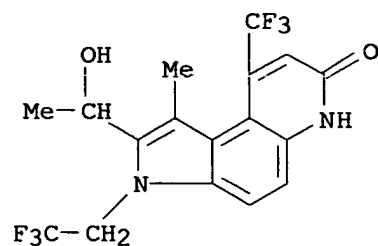
RN 453592-71-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-1-(hydroxymethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-72-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-hydroxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



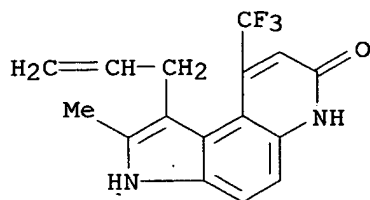
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 453593-32-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(androgen receptor modulator; preparation of pyrroloquinolines, pyridoquinolines, pyranoquinolines, and related tricyclic compds. as androgen receptor modulators)

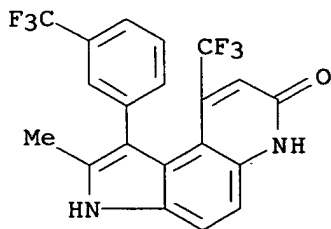
RN 453592-21-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-1-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-23-9 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

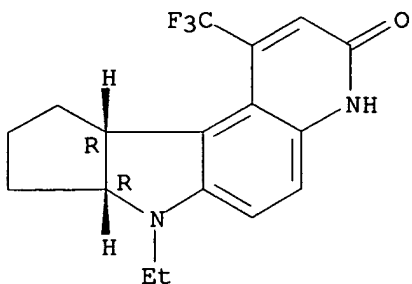


RN 453592-28-4 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-ethyl-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

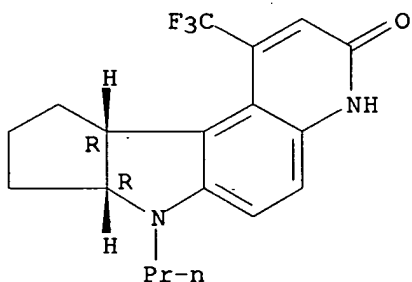
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RN 453592-32-0 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,10a-hexahydro-7-propyl-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

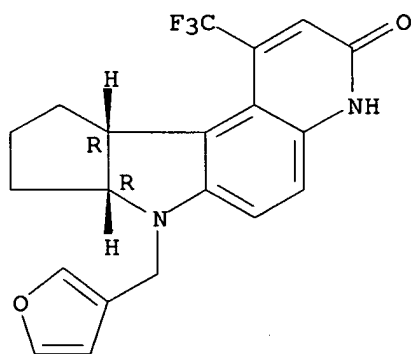
Relative stereochemistry.



RN 453592-33-1 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(3-furanylmethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

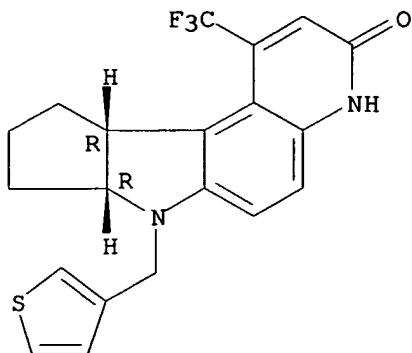


RN 453592-34-2 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(3-thienylmethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

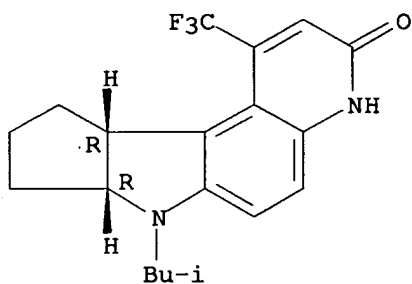
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RN 453592-35-3 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2-methylpropyl)-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

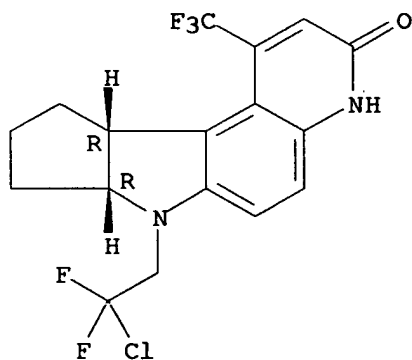
Relative stereochemistry.



RN 453592-36-4 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2-chloro-2,2-difluoroethyl)-7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

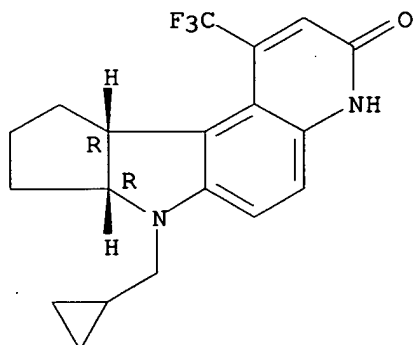


RN 453592-37-5 CAPLUS

10080926

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(cyclopropylmethyl)-
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INDEX NAME)

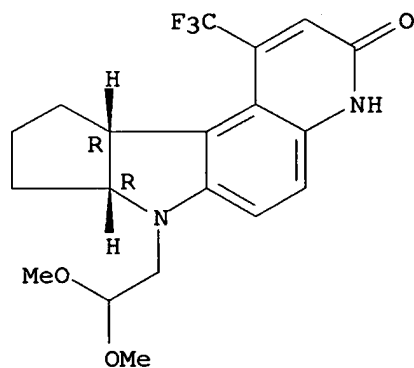
Relative stereochemistry.



RN 453592-38-6 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7-(2,2-dimethoxyethyl)-
7,7a,8,9,10,10a-hexahydro-1-(trifluoromethyl)-, (7aR,10aR)-rel- (9CI) (CA
INDEX NAME)

Relative stereochemistry.

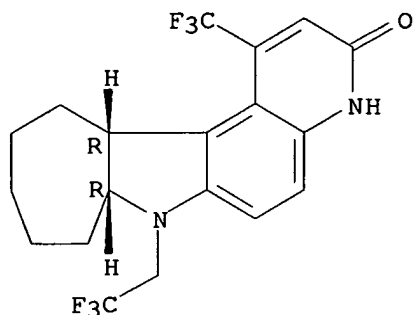


RN 453592-40-0 CAPLUS

CN Cyclohepta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,7a,8,9,10,11,12,12a-
octahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)-, (7aR,12aR)-rel-
(9CI) (CA INDEX NAME)

Relative stereochemistry.

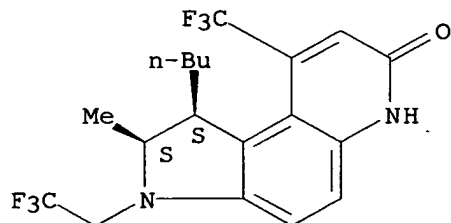
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RN 453592-42-2 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-butyl-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

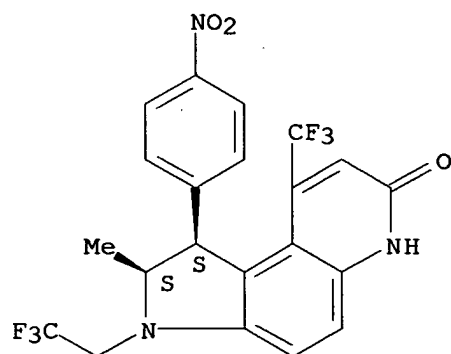
Relative stereochemistry.



RN 453592-43-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-nitrophenyl)-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

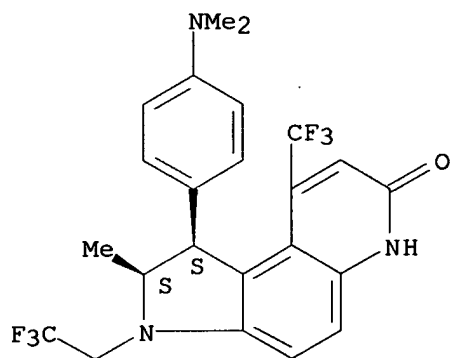


RN 453592-44-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[4-(dimethylamino)phenyl]-1,2,3,6-tetrahydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

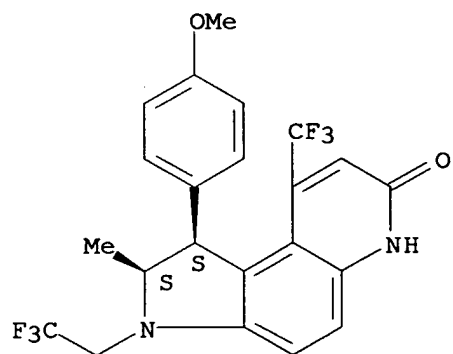
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RN 453592-45-5 CAPLUS

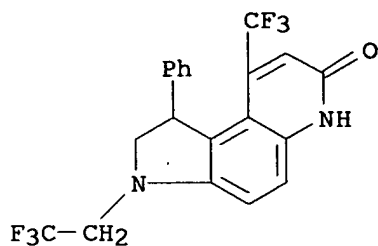
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



RN 453592-48-8 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-phenyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

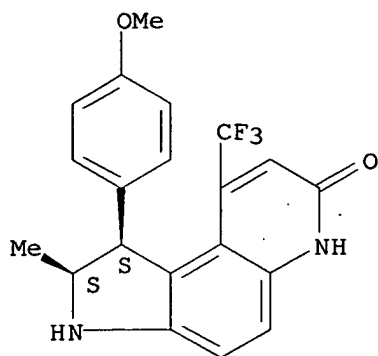


RN 453592-49-9 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

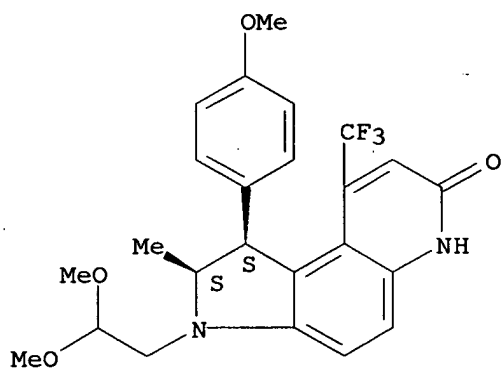
10080926



RN 453592-50-2 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-dimethoxyethyl)-1,2,3,6-tetrahydro-1-(4-methoxyphenyl)-2-methyl-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

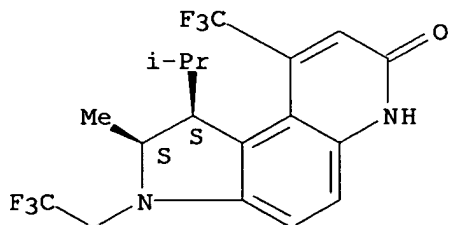
Relative stereochemistry.



RN 453592-51-3 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-methyl-1-(1-methylethyl)-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

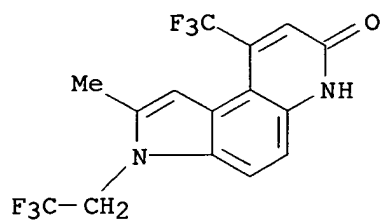
Relative stereochemistry.



RN 453592-59-1 CAPLUS

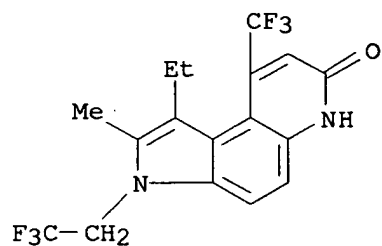
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



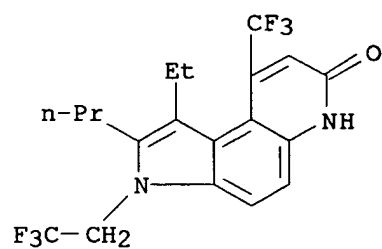
RN 453592-61-5 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-62-6 CAPLUS

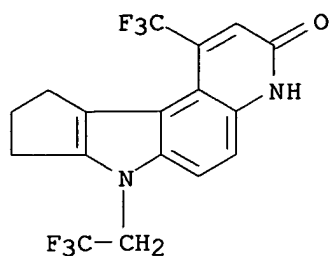
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-ethyl-3,6-dihydro-2-propyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-63-7 CAPLUS

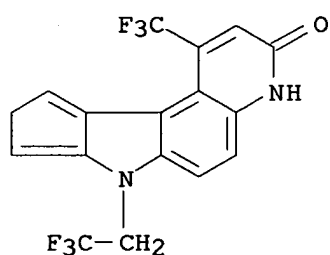
CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,8,9,10-tetrahydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



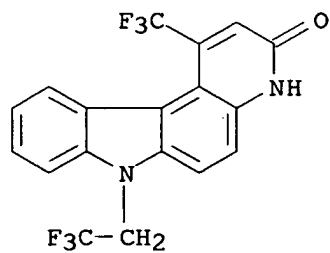
RN 453592-64-8 CAPLUS

CN Cyclopenta[4,5]pyrrolo[3,2-f]quinolin-3(4H)-one, 7,9-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-65-9 CAPLUS

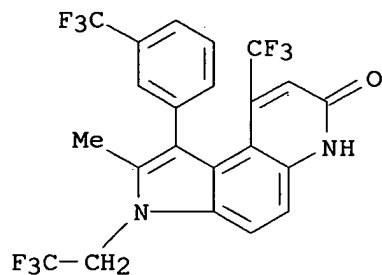
CN 3H-Pyrido[2,3-c]carbazol-3-one, 4,7-dihydro-7-(2,2,2-trifluoroethyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-67-1 CAPLUS

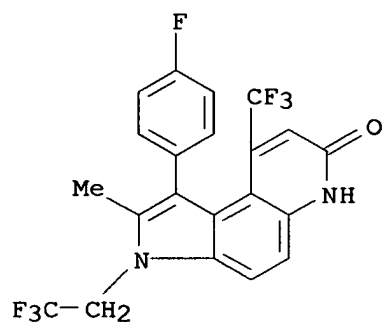
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

10080926



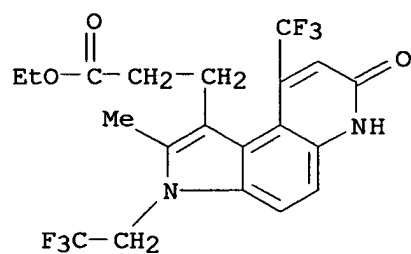
RN 453592-68-2 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(4-fluorophenyl)-3,6-dihydro-2-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-69-3 CAPLUS

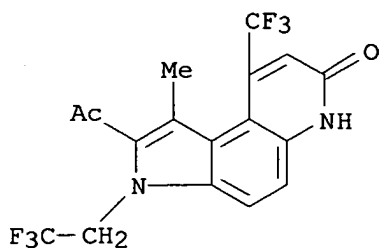
CN 3H-Pyrrolo[3,2-f]quinoline-1-propanoic acid, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 453592-73-9 CAPLUS

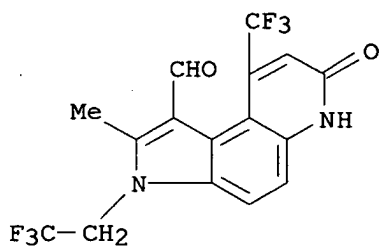
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-acetyl-3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



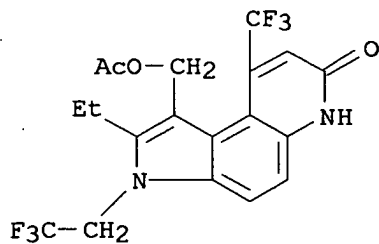
RN 453592-74-0 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinoline-1-carboxaldehyde, 6,7-dihydro-2-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



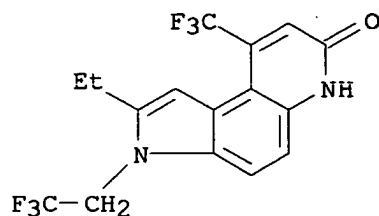
RN 453592-75-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-[(acetyloxy)methyl]-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-77-3 CAPLUS

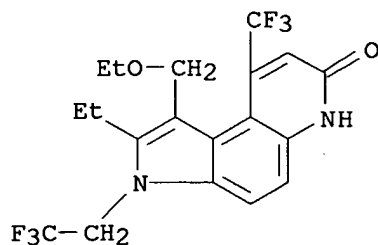
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



10080926

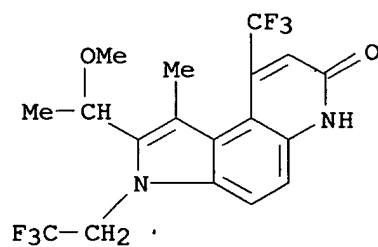
RN 453592-78-4 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1-(ethoxymethyl)-2-ethyl-3,6-dihydro-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



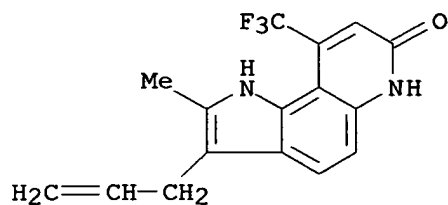
RN 453592-79-5 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2-(1-methoxyethyl)-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-80-8 CAPLUS

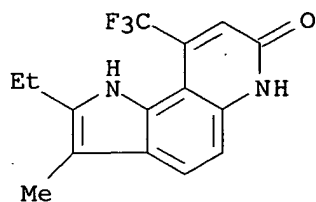
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-3-(2-propenyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453592-82-0 CAPLUS

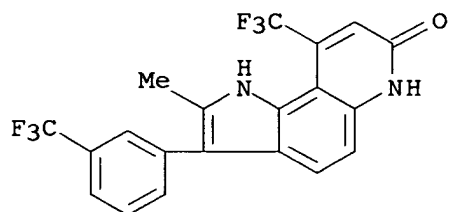
CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 2-ethyl-1,6-dihydro-3-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



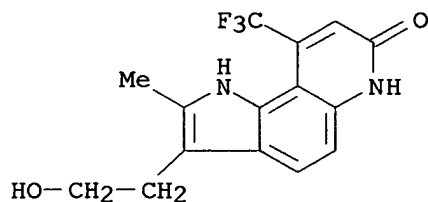
RN 453592-83-1 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2-methyl-9-(trifluoromethyl)-3-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



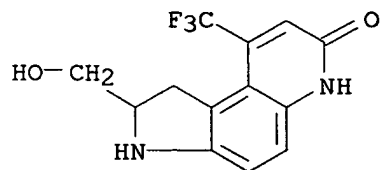
RN 453592-84-2 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-3-(2-hydroxyethyl)-2-methyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453593-25-4 CAPLUS

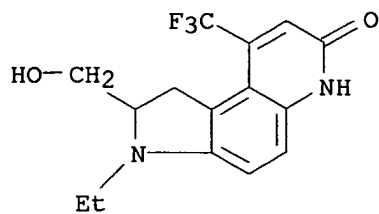
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 453593-26-5 CAPLUS

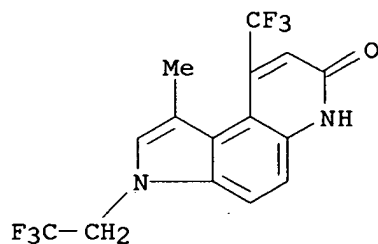
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-ethyl-1,2,3,6-tetrahydro-2-(hydroxymethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10080926



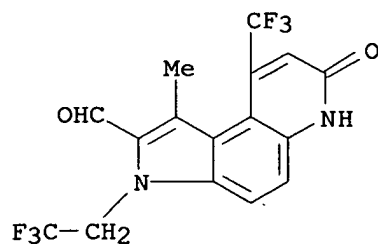
RN 453593-30-1 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1-methyl-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



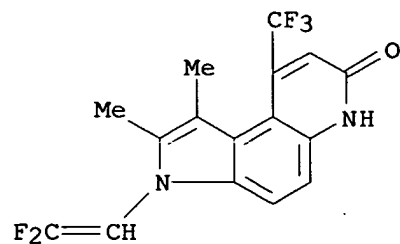
RN 453593-31-2 CAPLUS

CN 3H-Pyrrolo[3,2-f]quinoline-2-carboxaldehyde, 6,7-dihydro-1-methyl-7-oxo-3-(2,2,2-trifluoroethyl)-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)

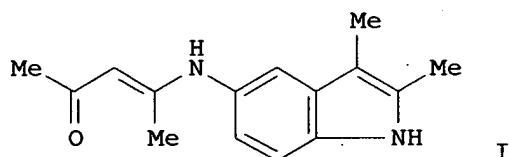


RN 453593-32-3 CAPLUS

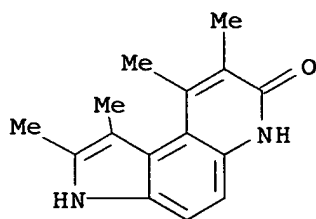
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3-(2,2-difluoroethenyl)-3,6-dihydro-1,2-dimethyl-9-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:455695 CAPLUS
 DN 131:213835
 TI Reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of
 pyrroloquinolines
 AU Yamashkin, S. A.; Trushkov, I. V.; Tomilin, O. B.; Terekhin, I. I.;
 Yurovskaya, M. A.
 CS Mordovian State Pedagogical Institute, Saransk, 430007, Russia
 SO Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya
 Geterotsiklicheskikh Soedinenii) (1999), Volume Date 1998, 34(9),
 1050-1065
 CODEN: CHCCAL; ISSN: 0009-3122
 PB Consultants Bureau
 DT Journal
 LA English
 GI

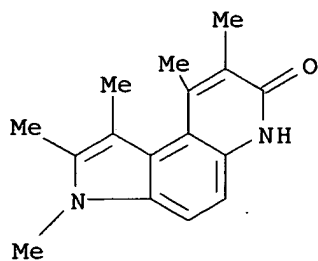


AB The concept of regioorientation is proposed for the annelation of the
 pyridine ring with the participation of 5-, 6-, and 7-aminoindoles (e.g.
 ,I). The conclusions based on the exptl. data are supported by
 semiempirical AML, PM3, and MNDO quantum-chemical calcns.
 IT **243669-00-3 243669-02-5 243669-06-9**
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
 nonpreparative)
 (reactivities of 5-, 6-, and 7-(enamino)indoles in the synthesis of
 pyrroloquinolines)
 RN 243669-00-3 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,8,9-tetramethyl- (9CI)
 (CA INDEX NAME)

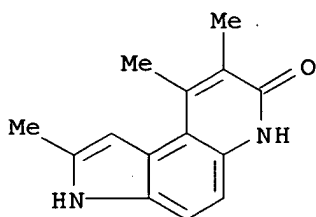


RN 243669-02-5 CAPLUS
 CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,3,8,9-pentamethyl- (9CI)
 (CA INDEX NAME)

10080926

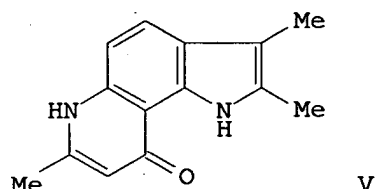
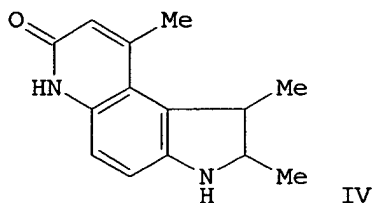
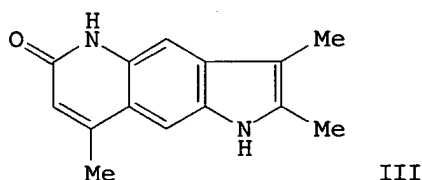
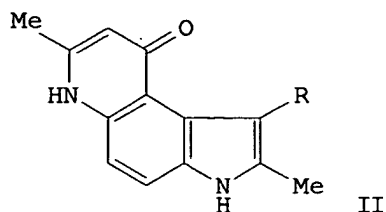
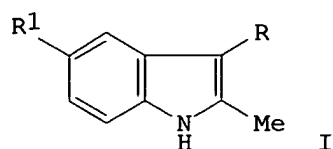


RN 243669-06-9 CAPLUS
CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-2,8,9-trimethyl- (9CI) (CA
INDEX NAME)



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:438395 CAPLUS
DN 99:38395
TI Synthesis of pyrroloquinolones
AU Yamashkin, S. A.; Yudin, L. G.; Kost, A. N.
CS Mosk. Gos. Univ., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1983), (4), 493-7
CODEN: KGSSAQ; ISSN: 0453-8234
DT Journal
LA Russian
OS CASREACT 99:38395
GI



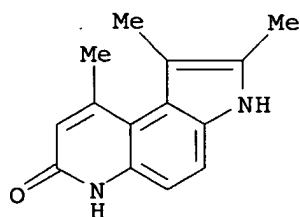
AB Intramol. cyclocondensation of I (R = Me, H; R1 = EtO2CCH:CMenH) by refluxing in biphenyl gave 89 and 95% pyrroloquinolines II. Similarly, refluxing I (R = Me, R1 = MeCOCH2CONH) in F3CCO2H gave a mixture containing III and IV. Refluxing I (R = Me, R1 = EtO2CCH:CMenH in the 6 position) with biphenyl gave 90% V.

IT **86269-88-7P 86269-91-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

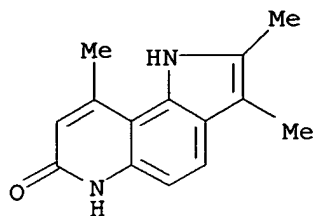
RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA INDEX NAME)



RN 86269-91-2 CAPLUS

CN 7H-Pyrrolo[2,3-f]quinolin-7-one, 1,6-dihydro-2,3,9-trimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1948:32006 CAPLUS

DN 42:32006

OREF 42:6783h-i,6784a-i,6785a-i,6786a-i,6787a-i,6788a-e

TI Orienting experiments on the reaction mechanism of aromatic bicyclic compounds

AU Huisgen, Rolf

CS Univ. Munich, Weilheim, Germany

SO Ann. (1948), 559, 101-52

DT Journal

LA Unavailable

OS CASREACT 42:32006

GI For diagram(s), see printed CA Issue.

AB A comprehensive monograph dealing largely with the theory of the reaction mechanism of naphthalene (I) and divided into the following parts: 1) static fixation of the double bonds in I; 2) fusion of a 3rd ring to derivs. of I; 3) structure of the I nucleus and the manner in which it reacts; 4) anellation and excitation structures in the I series; 5) naphthalenoid and benzenoid bicyclic compds.; 6) manner in which quinoline (II) and 1-hydroxyquinoline (III) react; 7) reactivity of aromatic polycyclic compds. (much of which involves the critical evaluation of previous work); and 8) an extensive exptl. part. The reactions of bicyclic compds. are discussed at length in terms of quantum-mech. calcns. of resonance energies (cf. Pauling and Wheland, C.A. 27, 3877; Sherman, C.A. 28, 6631.3; and Penney, C.A. 31, 2513.2). The hypothesis formulated by Marckwald (Ber. 23, 1015 (1890)) that the double bonds in I remain fixed loses its significance when anellation reactions (involving a 3rd ring) are considered. Previously the assumption was made that an "angular" tricyclic compound (IV) was normally formed. This was shown to be true in the case of 1-bromo- or 1-nitro-2-naphthylamine, either of which lose the 1-substituent on further cyclization to form the angular benzoquinoline. However, H. has shown that under certain conditions, a linear tricyclic form (V) may result. When 2 g. 1,2-MeClOH6NHAc (VI), m. 193°, was refluxed gently 5 hrs. with 2 g. arsenious acid, 7 g. glycerol, 7 g. H2SO4, and 5 g. AcOH, followed by treatment with 15 cc. H2O, digestion with NH4OH-CHCl3, filtration, evaporation of the CHCl3 extract, digestion with 8 g. Ac2O, saturation with NH4OH, reextn. with CHCl3, and treatment with 2 N HCl, H. obtained (after removal of residual VI, retreatment with NH4OH-CHCl3, and filtration through Al2O3) 0.53 g. 8-methyl-6,7-benzoquinoline (VII), b12 200°, m. 53-4° (not recrystd. due to high solubility in organic solvents); picrate, triclinic orange

prisms (from MeOH), m. 212° (decomposition). The mother liquors gave no trace of the known "angular" 5,6-benzoquinoline (VIII) (picrate, m. 254°). The HCl salt (IX) of VII forms golden yellow needles. The yellow perchlorate and orange-red nitrate of VII contrast sharply with the corresponding colorless salts of VIII. In ultraviolet light, VII in Me2CO shows intense light blue, and IX a pale yellow fluorescence. On the other

hand, VIII in organic solvents shows a very slight blue and its HCl salt gives a stronger blue fluorescence. 1,2-MeC₁₀H₆NHCOCH₂Ac (cf. Limpach, C.A. 25, 3999), m. 135°, (0.25 g.) was shaken with 2.5 cc. concentrated H₂SO₄, allowed to stand 1 hr., poured into ice-H₂O, made alkaline with NH₄OH, extracted with CHCl₃, evaporated, and taken up in MeOH, yielding 0.16 g. 2-hydroxy-4,8-dimethyl-6,7-benzoquinoline, pale yellow (sublimable) needles, m. 253°, insol. in aqueous alkaline solns. and in aqueous acids, but soluble in concentrated H₂SO₄ with a yellow color and yellowish green

fluorescence,

and giving a blue-green ultraviolet fluorescence in MeOH. On the other hand the "angular" 4-methyl-5,6-benzocarbostyryl shows practically no ultraviolet fluorescence in MeOH and a deep violet fluorescence in H₂SO₄.

Very similarly 0.35 g. 1,2-BrC₁₀H₆NHCOCH₂Ac, m. 117°, in H₂SO₄ was cyclized to 0.225 g. 2-hydroxy-4-methyl-8-bromo-6,7-benzoquinoline, pale yellow needles, m. 232-4°. From 2 g. 1,2-MeC₁₀H₆NH₂ and 1.6 g.

AcCH₂CO₂Et, H. obtained 2.5 g. 1-MeC₁₀H₆NHCMe:CHCO₂Et, m. 86-7° (from MeOH), 1.5 g. of which, gradually added to 20 g. paraffin oil at 270°, followed by heating 10 min. at 280°, gave 0.85 g.

"linear" 2,8-dimethyl-4-hydroxy-6,7-benzoquinoline, yellow needles, m. 340° (decomposition) (after successive crystns. from C₆H₆, PhNO₂, and EtOH), very soluble in 2 N NaOH, slightly soluble in hot 2 N HCl, showing

marked

blue-green ultraviolet fluorescence in NaOH, blue in NaOH, and yellowish green in concentrated H₂SO₄. From 0.3 g. 2-C₁₀H₇NHNH₂.HCl in 4 cc. MeOH with 0.2 cc. cyclohexanone, H. obtained a nearly quant. yield of 5,6-benzo-1,2,3,4-tetrahydrocarbazole (X), m. 137° (from MeOH); dark brown picrate, m. 192° (from C₆H₆). The formation of X is expedited by adding 2 N HCl to the original reaction mixture

1,2-MeC₁₀H₆NHAc, m. 193°, was hydrolyzed with HCl in alc. and 3.5 g. of the resulting salt in 25 cc. 7 N HCl was treated at 0° in 8 cc. H₂O with 1.34 g. NaNO₂, followed by treatment with urea and addition to 12 g. SnCl₂ in 8 cc. HCl and 110 cc. H₂O, giving a nearly quant. yield of 1-methyl-2-hydrazinonaphthalene-HCl (XI), leaflets (from HCl), m. 195° (decomposition), converted by AcONa into the free base, m. 110° (from MeOH), reducing Fehling solution XI with Me₂CO gave

2,1-Me₂C:NNHC₁₀H₆Me, leaflets, m. 99°. By heating 0.85 g. XI in 2 cc. AcOH with 1 cc. cyclohexanone and 20 mg. NiCl₂ 2 hrs. at 180°, and then 3 hrs. at 200°, a small amount of X was obtained, showing that ring closure had removed the 1-Me group. Careful warming of 135g. 3,6-(H₂N)(O₂N)C₆H₃Me with 125 g. arsenic acid, 270 g. glycerol, and 250 g. H₂SO₄ about 6 hrs. gave 108 g. of a difficultly separated mixture of 6-nitro-7-methylquinoline (XII) and its 5-Me isomer (XIII), from which 11.4 g. XIII, m. 165° (colorless HCl salt), was separated by successive crystns. from MeOH and Me₂CO. Inasmuch as the components in the mother liquors from XIII could not be fractionally crystallized, the solution was

evaporated,

treated with 350 cc. MeOH, and shaken 40 min. with 180 cc. hot 20% KOH in MeOH, followed by the addition of 700 cc. MeOH, yielding a highly insol. conversion product of XIII, the filtrate and washings from which gave 54 g. pure XII, colorless needles (from EtOH), m. 140°; colorless HCl salt. SnCl₂ reduction of XIII yielded 6-amino-5-methylquinoline, coarse prisms, m. 163-4° (from C₆H₆) (yellow HCl salt; Ac derivative m. 168°), which when diazotized and poured into a Cu₂O suspension in EtOH gave 5-methylquinoline, pale yellow oil (picrate m. 213-14°) (cf. Skraup and Brunner, Monatsh. 7, 141(1886)), 0.43 g. of which after treatment 10 hrs. with 0.65 g. CrO₃ and 5 cc. 35% H₂SO₄ gave 5-carboxyquinoline, m. 330° (cf. Yakubovich, C.A.5,503). By a similar series of reactions XII gave the following: 6-amino-7-methylquinoline, plates, m. 139° (from C₆H₆); 7-methylquinoline (picrate, m. 235°, identical with that prepared from 3-MeC₆H₄NH₂ by

the Skraup synthesis); 7-carboxyquinoline, m. 245°. XIII (1 g.) heated at the b.p. 3 min. with 12 cc. 10% KOH in MeOH gave 0.79 g. 1,2-bis(6-nitro-5-quinolyl)ethane, m. 300° (decomposition) (from AcOH), also formed when 2 N NaOH or alkaline arsenite solns. are used in place of KOH. The corresponding diamine, C₂₀H₁₈N₄, formed greenish yellow needles (from C₆H₆) (properties not given). By analogous procedures H. obtained from 6-nitro-5,8-dimethylquinoline 1,2-bis(6-nitro-8-methyl-5-quinolyl)ethane, nearly colorless needles, m. 257° (from pyridine or AcOH), and from 5-nitro-8-methylquinoline 1,2-bis(5-nitro-8-quinolyl)ethane, needles, m. 221° (from C₆H₆ or AcOH), which on further treatment with alkali gave a deep violet color (cf. Trautmann, Ber. 23, 3673(1890)). 2-O₂NC₆H₄Me in cooled absolute Et₂O, treated with an equimol. amount of alc.-free EtOK in Et₂O, the mixture let stand overnight, shaken with H₂O, and the Et₂O layer dried, filtered through Al₂O₃, and concentrated, gave 25-30% o,o'-dinitrobibenzyl, needles (from MeOH), m. 122°. Knuppel's reaction (cf. Ann. 310, 75(1900)), in which 6-nitroquinoline was heated with MeONa, gave 80% of a quinazone N-oxide (XIV), yellow needles, decomposing 330° (from AcOH) (red HCl salt (from H₂O)), which when distilled with Fe powder gave the O-free quinazone, C₁₈H₁₀N₄, pale yellow leaflets (from C₆H₆), m. 369°, sublimes undecompd. at 400°, gives a colorless HCl solution, and when heated with Zn dust, yields a bluish green semiquinone-like compound that may be reoxidized to the original quinazone by KMnO₄. A reaction analogous to that giving XIV yielded from XII the 7,7'-di-Me derivative, yellow needles (from AcOH), m. 355° (decomposition), yielding, on reduction, the dimethylquinazone, C₂₀H₁₄N₄, long, pale yellow needles, m. 380° (from xylene). Similarly 6-nitro-7,8-dimethylquinoline gave the corresponding tetra-Me derivative of XIV, yellowish green needles (from PhNO₂), decomposing above 330° and forming, when distilled with Fe, the tetramethylquinazone, pale yellow needles, m. 354°.

6-Nitroquinoline (1 g.), 0.5 g. KCN, 15 cc. EtOH, 3 cc. H₂O, and 0.5 g. KOH heated 4 hrs. gave 0.5 g. 5-cyano-6-ethoxyquinoline, needles, m. 130° (from MeOH), very resistant to HNO₂, hot concentrated HCl, and cold H₂SO₄, whose colorless HCl and H₂SO₄ salts are difficultly soluble in H₂O. By a similar reaction, using MeOH in place of EtOH, 5-cyano-6-methoxyquinoline, needles (from MeOH), m. 179°, was obtained. To a cooled mixture of 5 g. 6-nitroquinoline, 6 g. HONH₂.HCl, and 90 cc. EtOH was added (in 1 portion) 30 cc. 20% KOH in MeOH. The exothermic reaction gave rise to 94% 5-amino-6-nitroquinoline (XV), yellow needles, m. 272° (yellow, difficultly soluble HCl salt), which with SnCl₂ in HCl gave 5,6-diaminoquinoline chlorostannate; the latter, after detinning with H₂S, yielded the HCl salt, pale yellow crystals, 0.1 g. of which when heated with 0.12 g. benzil in 5 cc. alc. and small amts. of AcONa gave the substituted quinoxaline, C₂₃H₁₅N₃ (0.88 g.), plates from C₆H₆, m. 205°; the di-Ac derivative m. 252° with decomposition to form 5,6-(methylimidazolo)quinoline, m. 200° (hydrate, m. 70°). The latter was more readily prepared by heating 0.5 g. XV in 5 cc. AcOH several hrs. with 2.1 g. SnCl₂ in 4 cc. HCl, followed by detinning, evaporation, treatment with NH₄OH, and extraction with Me₂CO. Similarly, when

XV

was reduced in the presence of HCO₂H (instead of AcOH), 5,6-imidazoloquinoline, m. 214° (from C₆H₆) (hydrate, m. 78°), was formed. By diazotization, the NH₂ group in XV was replaced by iodine (using KI and Cu-bronze), yielding a resin which after trituration with HCl, extraction with NH₄OHCHCl₃, followed by washing with

aqueous

Na₂SO₄ and H₂O, and passing the CHCl₃ solution through Al₂O₃, gave red needles, which on repeated crystallization from MeOH and C₆H₆ yielded colorless 5-iodo-6-chloroquinoline, m. 136°. Deiodination with Cu-bronze in boiling PhNO₂ gave 6,6'-dichloro-5,5'-biquinoline, colorless polyhedrons,

m. 205°. When, however, the iodine was removed by means of HI in AcOH, 5-iodo-6-chloroquinoline gave 6-chloroquinoline, m. 40-1°. Skraup's cyclization of 0.5 g. 5-nitro-6-aminoquinoline (Kaufmann and Zeller, C.A. 12, 1390), using arsenic acid gave 0.115 g. 4,7-phenanthroline, polyhedrons (from C₆H₆), m. 174° (showing only a faint ultraviolet fluorescence), also obtained (in 65% yield) by cyclization of 5-bromo-6-aminoquinoline. Evidently NO₂ or Br in position 5 fails to block the formation of 4,7-phenanthroline. On the other hand, when 1 g. 6-acetamido-5-methylquinoline was heated gently 10-12 hrs. with 0.9 g. arsenic acid, 6 g. glycerol, 6 g. H₂SO₄, and 5 g. glacial AcOH, followed successively by treatment with H₂O, extraction with NH₄OH-CHCl₃, extraction

with 2 N HCl, reextrn. with NH₄OH-CHCl₃, evaporation, treatment of the dry extract

with 3 cc. pyridine and 0.2 g. 4-MeC₆H₄SO₂Cl (to remove any unchanged starting product), and continued purification by extracting alternately with alkaline CHCl₃ and HCl, filtering the CHCl₃ solution through Al₂O₃, and finally subjecting the product to microdistn., using a water pump, H. obtained 3 fractions: (a) subliming 180°, (b) yellow oil, b. 200-20°, and (c) a red oil, b. 235°. Of these (b) gave 12 mg. linear 10-methyl-1,5-anthrazoline hydrate, C₁₅H₁₀N₂·3H₂O, felted needles, m. 62°, giving a yellow solution in acids and showing a brilliant bluish violet (ultraviolet) fluorescence. 8-Methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline (XVI), m. 225-6° (from EtOH), was prepared in 70% yield by heating 0.5 g. 6-hydrazino-8-methylquinoline (the synthesis of which is not given) with 3 cc. AcOH and 1.5 cc. cyclohexanone 6 hrs. and purifying the product by methods similar to those given above. XVI was also readily obtained in 75% yield by heating 0.33 g. of the substituted cyclohexanone hydrazone (XVII), m. 189°, at 200-240° with 15 mg. dry NiCl₂, or (in only 34% yield) by heating this same hydrazone with 2 N H₂SO₄. The following steps also led to the formation of XVI: 4-nitro-2,5-xylylidine → Skraup's synthesis 50% 6-nitro-5,8-dimethylquinoline, m. 118° (from alc.) → SnCl₂ 6-amino derivative, b. 12 194°, prisms, m. 175° → HCl salt, yellow → 7 N HCl+HNO₂ diazo derivative → SnCl₂ chlorostannate → H₂S+HCl 85% 6-hydrazino-5,8-dimethylquinoline-HCl, yellow needles (free base (XVIII), m. 185°) → cyclohexanone 30% XVI. The ultraviolet absorption spectra of XVI prepared by the various methods were identical and showed a striking similarity to that of 7,8-dimethyl-10,11-tetramethylene-5,6(N)-pyrroquinoline. XVIII fails to undergo cyclization to XVI unless HCl is present. 6-Hydrazino-8-methylquinoline-HCl and MeCOEt in AcOH gave 40% 8,10,11-trimethyl-5,6(N)-pyrroquinoline, m. 188° (from EtOH), also formed in poor yield from the HCl salt of XVIII with concomitant removal of a Me group. Similarly, 0.5 g. 5-hydrazinoquinoline-HCl and cyclohexanone in AcOH gave 0.42 g. 10,11-tetramethylene-5(N),6-pyrroquinoline (XIX), m. 289° (from Me₂CO). XIX was also isolated in 1-2% yield after extensive purification from 5-hydrazino-6-methylquinoline, m. 158° (pale yellow HCl salt).

SnCl₂ reduction of 15 g. 6-nitro-2-hydroxylepidine gave 9.6 g. 2-hydroxy-4-methyl-6-aminoquinoline (XX), pale yellow, m. above 300°, cyclizing in the presence of arsenic acid, glycerol, and H₂SO₄-AcOH, followed by successive treatments with HCl and NH₄OH, to form 2-hydroxy-4-methyl-4,7-phenanthroline (XXI), colorless prisms, the "angularity" of which was attested to by its very faint ultraviolet fluorescence, its ready solubility in aqueous NaOH and in boiling aqueous

Na₂CO₃, and

by the fact that its salts are colorless. 2,5-Xylylidine, when heated at 160° with an equimol. amount of AcCH₂CO₂Et, gave the N-acetylacetyl derivative, m. 96° (from aqueous MeOH), which when heated 0.5 hr. on a steam bath with 6 parts concentrated H₂SO₄ gave (after pouring on ice) 90%

2-hydroxy-4,5,8-trimethylquinoline, m. 238° (from EtOH); 6-nitro derivative, pale yellow, m. 275° (from AcOH or EtOH); 6-amino derivative (XXII) (formed from the orange-red Sn double salt), pale yellow leaflets, m. 302° (from aqueous NH₄OH or EtOH) (colorless HCl salt, difficultly soluble in H₂O). The Skraup cyclization of XXII gave 2-hydroxy-4,9,10-trimethyl-1,5-anthrazoline (XXIII), pale yellow needles (from glacial AcOH or Ac₂O), m. 290°, whose linear structure was indicated by the yellow color of its acid solns., its insoly. in alkali, and its strong blue ultraviolet fluorescence in MeOH. On diazotization, followed by SnCl₂ reduction, XX gave 90% 2-hydroxy-4-methyl-6-hydrazinoquinoline, colorless needles from H₂O, decomposing 240°, reducing Fehling solution in the cold, and forming a colorless HCl salt, which, when cyclized in the presence of MeCOEt and glacial AcOH, gave 90% 2-hydroxy-4,10,11-trimethyl-5,6(N)-pyrroquinoline, needles (from alc.), m. above 300° (decomposition); yellow HCl salt. When an analogous cyclization was carried out in the presence of cyclohexanone, 2-hydroxy-4-methyl-10,11-tetramethylene-5,6(N)-pyrroquinoline, m. above 300°, was formed; golden yellow HCl salt. Diazotization of XXII, followed by reduction, gave the yellow chlorostannate of 2-hydroxy-4,5,8-trimethyl-6-hydrazinoquinoline, which in hot H₂O, followed by filtration of the stannic acid, reacted with MeCOEt to form the corresponding substituted hydrazone, pale yellow needles, m. 112° (from a buffered AcONa solution), which failed to cyclize when treated with ZnCl₂ at 200-60°, giving only 4,5,8-trimethylcarbostyryl, m. 236°. Other attempts to cyclize the compound were equally unsuccessful. 2,3-Diphenyl-4,5-benzoindeole, colorless prisms with blue-green iridescence, m. 166-7°, (3 g.) was formed from 1 g. 2-H₂NC₁₀H₇, 0.5 g. C₁₀H₇NH₂.HCl, and 2.2 g. benzoin at 140-65° (cf. Japp and Murray, J. Chemical Society 65, 889(1894)). 2,1-H₂NC₁₀H₆Me subjected to a similar reaction gave 1-methyl-2-desylaminonaphthalene, 2,1-[PhC(OH):CPhNH]C₁₀H₆Me, pale yellow, m. 152-3° (from CHCl₃-MeOH), which could not be cyclized by the use of ZnCl₂, H₂SO₄, H₃PO₄, SnCl₄, NiCl₂, or SOCl₂. The structure of this compound was shown by HClMeOH hydrolysis to benzoin and 2,1-H₂NC₁₀H₆Me. The resonance energy of I was calculated from the total hydrogenation to decahydronaphthalene and also from its partial hydrogenation to tetrahydronaphthalene. The values obtained were, resp., 63.5 and 63.1 kcal./mol. and the approx. resonance energy per ring was 31.5 kcal. (cf. also Pauling, "Nature of the Chemical Bond," C.A. 33, 6700.4).

IT 86269-88-7, 3H-Pyrrolo[3,2-f]quinolin-7-ol, 1,2,9-trimethyl-
(preparation of)

RN 86269-88-7 CAPLUS

CN 7H-Pyrrolo[3,2-f]quinolin-7-one, 3,6-dihydro-1,2,9-trimethyl- (9CI) (CA
INDEX NAME)

